

STRUCTURES OF SUBSTRATE BINDING POCKETS OF SCF COMPLEXES

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FIELD OF THE INVENTION

The present invention relates to binding pockets of Skp1-Cdc53/Cullin-F-box protein (SCF) E3 ubiquitin ligases associated with substrate selection and/or orientation. In particular, the invention relates to a crystal comprising such binding pockets. The crystal may be useful for modeling and/or synthesizing mimetics of a binding pocket or ligands that associate with the binding pocket. Such mimetics or ligands may be capable of acting as modulators of the interactions of an SCF E3 ubiquitin ligase and its substrates, and they may be useful for treating, inhibiting, or preventing diseases modulated by such interactions.

Methods are also provided for regulating an SCF E3 ubiquitin ligase comprising changing a binding pocket associated with substrate selection and/or orientation.

BACKGROUND

The ubiquitin proteolytic system controls the precisely timed degradation of regulatory proteins in signaling, development and cell cycle progression. Substrate ubiquitination is catalyzed by a cascade of enzymes, termed E1, E2 and E3, which activate and then conjugate ubiquitin to the substrate (Hershko and Ciechanover, 1998). E3 enzymes, also known as ubiquitin ligases, contain substrate-specific recognition domains and catalyze the final step in ubiquitin transfer. Recognition is mediated by primary sequence elements in the substrate, referred to as degrons (Varshavsky, 1991). Control of the E3-substrate interaction forms the basis for regulated proteolysis; often post-translational substrate modification, most commonly phosphorylation, serves to target substrates to their cognate E3 enzymes (Deshaies, 1999). Two main classes of E3 enzyme are now evident, as characterized by the presence of either a HECT domain or a RING domain. The HECT domain class forms a catalytically essential thioester with ubiquitin, whereas the RING domain class relies on the E2 enzymes to provide catalytic activity (Pickart, 2001). The RING domain forms an E2 docking site and orients the substrate with respect to the E2.

Phosphorylation-dependent degrons direct substrates to a recently described class of multisubunit E3 enzymes termed Skp1-Cdc53/Cullin-F-box protein (SCF) complexes. SCF complexes are built on an invariant core machinery comprised of the adapter protein Skp1, the scaffold protein Cdc53 (called Cul1 in metazoans), and the RING-H2 domain protein Rbx1 (also called Roc1 or Hrt1), which interacts with an E2 enzyme, usually Cdc34 (Pickart, 2001). Substrates are brought to the core complex by one of a large family of variable adapter subunits called F-box proteins, each of which targets a limited number of specific substrates (Bai et al., 1996, Patton et al., 1998). F-box proteins typically have a bipartite structure with an N-terminal ~40 amino acid F-box motif and a C-terminal protein-protein interaction domain, such as WD40 repeats or leucine rich repeats, which bind substrates (Bai et al., 1996; Feldman et al, 1997; Skowyra et al., 1997). The overall architecture of SCF complexes is conserved in several

related ubiquitin ligase complexes including the Anaphase Promoting Complex/Cyclosome and the Von Hippel Lindau (VHL) tumor suppressor protein complex, each of which contain cullin family members, RING-H2 domain and substrate recognition subunits (Pickart, 2001; Kaelin, 2002).

Cell cycle progression depends on the precisely timed elimination of cyclins and cyclin-dependent kinase (CDK) inhibitors by the ubiquitin system (Harper et al, 2002). In yeast, G1 cyclin CDK activity phosphorylates a CDK inhibitor called Sic1, whose degradation is necessary for onset of B-type cyclin CDK activity and DNA replication (Schwob et al., 1994). Phospho-Sic1 is specifically recognized by the F-box protein Cdc4, which recruits Sic1 for ubiquitination by the Cdc34-SCF complex (Bai et al., 1996; Feldman et al., 1997; Skowyra et al., 1997). Stable forms of Sic1 that lack CDK phosphorylation sites cause a G1 phase arrest (Verma et al., 1997), whereas deletion of *SIC1* causes premature DNA replication and rampant genome instability (Lengronne and Schwob, 2002). Cdc4 recruits several other substrates to the SCF core complex in a phosphorylation dependent manner, including the Cln-Cdc28 inhibitor/cytoskeletal scaffold protein Far1, the replication protein Cdc6 and the transcription factor Gcn4 (Patton et al., 1998). The F-box protein Grr1 functions in an analogous manner to render G1 cyclins unstable throughout the cell cycle, in a manner that depends on recognition of phospho-epitopes by the LRR domain of Grr1 (Skowyra et al, 1997; Hsiung et al, 2001).

In the metazoan cell cycle, SCF complexes target phosphorylated forms of the CDK inhibitor p27^{Kip1} and cyclin E, among other substrates. Interestingly, F-box protein specificity for these substrates is reversed compared to yeast, in that the WD40 domain of hCdc4/Fbw7/Ago/SEL-10 recognizes cyclin E (Strohmaier et al., 2001; Koepp et al., 2001; Moberg et al., 2001), whereas the LRR domain of Skp2 recognizes p27^{Kip1} in conjunction with the CDK-binding protein Cks1 (Harper, 2001). Both of these degradation pathways are perturbed in cancer cells. Many primary tumors express high levels of Skp2, which leads to premature degradation of p27^{Kip1} and cell cycle entry (Harper, 2001). Conversely, loss of Cdc4 function causes deregulation of cyclin E-CDK2 activity, which leads to precocious S phase entry and genome instability (Spruck et al., 1999). Mutations in the *Drosophila* homolog of *CDC4*, called *ago*, were isolated as homozygous recessive alleles in a screen for excess cell proliferation, a defect attributed to ectopic cyclin E activity (Moberg et al., 2001). Mutations in *hCDC4* have been detected in several cancer cell lines that exhibit high levels of cyclin E (Moberg et al., 2001; Strohmaier et al., 2001), as well as in a significant fraction of primary endometrial cancers (Spruck et al., 2002). In addition, *hCDC4* is located in the 4q32 region, which is often deleted in various cancers (Spruck et al., 2002). Significantly, a high level of cyclin E correlates strongly with low survival rates in breast cancer (Keyomarsi et al., 2002). Other important substrates appear to be targeted for degradation by Cdc4 orthologs in a phosphorylation-dependent manner, including activated forms of the developmental regulator Notch and the presenilins, which are implicated in familial early onset Alzheimer's disease (Lai, 2002; Selkoe, 2001). SCF-dependent proteolysis also mediates other important signaling events, including phosphorylation-dependent degradation of the NF κ B inhibitor I κ B α and the proto-oncogene product β -catenin by the F-box protein β -TrCP (Pickart, 2001).

Several F-box proteins can recognize short phosphopeptide motifs that correspond to substrate sequences. However, it is unknown whether such interactions are analogous to phosphorylation-dependent interactions of SH2, PTB, 14-3-3, WW and FHA domains, each of which has been crystallized with its cognate phosphopeptide (Yaffe and Elia, 2001). For many SCF substrates, including Sic1, Cdc6 and Cln2, phosphorylation on multiple dispersed sites is required for recognition and degradation (Patton et al., 1998). We recently defined a high affinity consensus phosphopeptide binding motif for Cdc4, termed the Cdc4 phospho-degron (CPD), which bears the consensus I/L-I/L/P-pT-P-<KR>₄ [SEQ ID NO:1], where < > indicates a disallowed residue (Nash et al., 2001). The P0 phospho-threonine residue, or less favorably a phospho-serine residue, and the P+1 proline are essential for interaction with Cdc4. Unexpectedly, the CPD consensus is at odds with the CDK phosphorylation site consensus, S/T-P-X-K/R [SEQ ID NO:2](Endicott et al., 1999). Thus, substrate recognition by the targeting kinase is counter-balanced against the targeting component of the degradation machinery. All nine CPD sites in Sic1 have one or more sub-optimal features: all lack consensus hydrophobic residues in the P-1 or P-2 positions, four have serine in place of threonine in the P0 position, and seven contain a disfavored basic residue in one of the +2 to +5 positions. Unexpectedly, Sic1 must be phosphorylated on at least six of its nine sites in order to allow recognition by Cdc4 (Nash et al., 2001). This requirement for multi-site phosphorylation in principle renders the rate of Sic1 degradation proportional to the sixth power of G1 CDK concentration (Ferrell, 1996). The inherently ultrasensitive nature of the Sic1 degradation reaction appears critical for the coordinated initiation of DNA replication by S phase CDK activity (Nash et al., 2001; Lengronne and Schwob, 2002).

The mechanism of the ubiquitin conjugation reaction is not well understood. The ability of E2-E3 enzyme complexes to form polymers of ubiquitin, itself an 8 kDa protein, on a protein substrate presumably demands a large catalytic cradle simply to accommodate the initial reactants (Pickart, 2001). The sequential addition of ubiquitin moieties onto the substrate must also entail considerable flexibility of the substrate and/or the enzyme complex in order to extend the ubiquitin chain. Recent structure determination and modeling of three E2-E3 complexes has provided insight into these issues. A complex of the E2 enzyme UbcH7 and the HECT domain enzyme E6AP reveals a distance of ~ 50Å between the E2 and E3 active sites, suggesting that catalytic transfer of ubiquitin requires large scale movements in an as yet undefined process (Huang et al., 1999). Similarly, a complex between UbcH7 and the RING domain E3 c-Cbl contains a substantial gap between the E2 active site and the substrate binding site on c-Cbl (Zheng et al., 2000). Structures of the SOCS-box adapter protein VHL in complex with a hydroxylated substrate peptide have recently been solved (Kaelin, 2002), but the orientation of the substrate binding site with respect to the E2 enzyme is unknown. Finally, structure determination and molecular modeling of the holo-SCF^{Skp2} complex again suggests a distance of ~ 50Å between the substrate binding LRR domain in Skp2 and the E2 active site (Zheng et al., 2002). Notably, the extensive interdigitation of the Skp1-Skp2 interface and the Skp2 inter-domain interface rigidly fixes the orientation of the LRRs of Skp2, suggesting that the F-box protein might hold the substrate in a very precise orientation with respect to the E2 enzyme (Schulman et al., 2000). However, because the substrate binding site on

Skp2 has not been determined, either by mutation or by co-crystallization with substrate peptide, it is not possible to deduce how SCF substrates might be positioned with respect to the E2 catalytic site.

SUMMARY OF THE INVENTION

Applicants have determined the structures of binding pockets of SCF E3 ubiquitin ligases involved in substrate recognition and/or orientation. More particularly, Applicants have solved the x-ray crystal structure of binding pockets of F-box proteins/ F-box protein-Skp1 complexes of SCF E3 ubiquitin ligases that interact with Cdc4 phospho-degron (CPD) motifs.

Solving the crystal structure has enabled the determination of key structural features of substrate binding pockets of a SCF E3 ubiquitin ligase, particularly the shape of binding pockets, or parts thereof, that permit association of a substrate with a SCF E3 ubiquitin ligase or part thereof. The crystal structure also enables the determination of key structural features in substrates or ligands that interact or associate with the binding pockets.

Knowledge of the structural features of substrate binding pockets of a SCF E3 ubiquitin ligase is of significant utility in drug discovery. The SCF E3 ubiquitin ligase substrate interaction is the basis of many biological mechanisms. In particular it is the basis for regulated ubiquitin proteolysis resulting in degradation of regulatory proteins involved in signaling, development, and cell cycle progression. In addition, drugs may exert their effects through association with the binding pockets of SCF E3 ubiquitin ligases. The associations may occur with all or any parts of a binding pocket. An understanding of the association of a drug with binding pockets of SCF E3 ubiquitin ligases will lead to the design and optimization of drugs having more favorable associations with their targets and thus provide improved biological effects. Therefore, information about the shape and structure of substrate binding pockets of SCF E3 ubiquitin ligases is invaluable in designing potential modulators of the SCF E3 ubiquitin ligases for use in treating diseases and conditions associated with or modulated by the SCF ubiquitin ligases, including cancer and Alzheimer's Disease.

The present invention relates to an isolated binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation. In an embodiment, the invention relates to a binding pocket of an F-box protein/F-box protein-Skp1 complex of a SCF E3 ubiquitin ligase that interacts with a Cdc4 phospho-degron (CPD) motif. In an aspect of the invention, the binding pocket regulates the binding of a CPD motif to a SCF E3 ubiquitin ligase.

In an embodiment, the invention comprises the structure of a WD repeat domain of an F-box protein. The structure may also comprise a helical linker of an F-box protein and optionally an F-box domain of an F-box protein. Still further the structure may comprise a Skp1 protein.

The invention also relates to a crystal comprising a binding pocket of a SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation.

In an embodiment, the invention provides a crystal comprising a WD repeat domain of an F-box protein. The crystal may also comprise a helical linker of an F-box protein and optionally an F-box domain of an F-box protein. Still further the crystal may comprise a Skp1 protein.

The present invention also contemplates molecules or molecular complexes that comprise all or parts of either one or more binding pockets of the invention, or homologs of these binding pockets that have similar structure and shape.

The invention also contemplates a crystal comprising a binding pocket of a SCF E3 ubiquitin ligase involved with substrate recognition and/or orientation in association with a substrate (e.g. CPD motif). A substrate may be complexed or associated with a binding pocket. The invention further contemplates a crystal comprising a binding pocket of a SCF E3 ubiquitin ligase involved with substrate recognition and/or orientation in association with a ligand. A ligand may be a modulator of the activity of a SCF E3 ubiquitin ligase. A ligand may be complexed or associated with a binding pocket

In an aspect the invention contemplates a crystal comprising a binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation complexed with a substrate from which it is possible to derive structural data for the substrate.

The shape and structure of a binding pocket may be defined by selected atomic contacts in the pocket. In an embodiment, the binding pocket is defined by one or more atomic interactions or enzyme atomic contacts as set forth in Table 3 or Table 4. Each of the atomic interactions is defined in Table 3 or Table 4 by an atomic contact (more preferably, a specific atom where indicated) on the F-box protein and by an atomic contact (more preferably a specific atom where indicated) on the substrate. The atomic interactions are also defined by an atomic contact on one portion of the F-box protein and an atomic contact on another portion of the F-box protein.

An isolated polypeptide comprising a binding pocket with the shape and structure of a binding pocket described herein is also within the scope of the invention.

The invention also provides a method for preparing a crystal of the invention, preferably a crystal of a binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation, or a complex of such a binding pocket and a substrate.

Crystal structures of the invention enable a model to be produced for a binding pocket of the invention, or complexes or parts thereof. The models will provide structural information about the interactions of a substrate or ligand with a binding pocket. Models may also be produced for substrates and ligands. A model and/or the crystal structure of the present invention may be stored on a computer-readable medium.

The present invention includes a model of a binding pocket of the present invention that substantially represents the structural coordinates specified in Table 6 or portions thereof. The invention also includes a model that comprises modifications of the structure substantially represented by the structural coordinates specified in Table 6. A model is a representation or image that predicts the actual structure of the binding pocket. As such, a model is a tool that can be used to probe the relationship between a binding pocket's structure and function at the atomic level, and to design molecules that can modulate the binding site and accordingly activity of an F-box protein or SCF complex.

Thus, the invention provides a model of: (a) a binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation; and (b) a modification of the model of (a).

A method is also provided for producing a model of the invention representing a binding pocket of an SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation, comprising representing amino acids of the binding pocket at substantially the structural coordinates specified in Table 6.

5 A crystal and/or model of the invention may be used in a method of determining the secondary and/or tertiary structures of a polypeptide or binding pocket with incompletely characterised structure. Thus, a method is provided for determining at least a portion of the secondary and/or tertiary structure of molecules or molecular complexes which contain at least some structurally similar features to a binding pocket of the invention. This is achieved by using at least some of the structural coordinates set out in Table 6.

10 A crystal of the invention may be useful for designing, modeling, identifying, evaluating, and/or synthesizing mimetics of a binding pocket or ligands or substrates that associate with a binding pocket. Such mimetics or ligands may be capable of acting as modulators of an F-box protein or SCF E3 ubiquitin ligase activity, and they may be useful for treating, inhibiting, or preventing diseases modulated by such a protein or ligase.

15 Thus, the present invention contemplates a method of identifying a modulator of a F-box protein or an SCF E3 ubiquitin ligase comprising the step of applying the structural coordinates of a binding pocket, or atomic interactions, or atomic contacts of a binding pocket, to computationally evaluate a test ligand or substrate for its ability to associate with the binding pocket, or part thereof. Use of the structural coordinates of a binding pocket, or atomic interactions, or atomic contacts of a binding pocket to design or identify a modulator is also provided.

20 In an embodiment, the invention contemplates a method of identifying a modulator of an F-box protein or an SCF E3 ubiquitin ligase comprising determining if a test agent inhibits or potentiates the interaction of an F-box protein or SCF E3 ubiquitin ligase with its substrate.

25 The invention further contemplates classes of modulators of F-box proteins or SCF E3 ubiquitin ligases based on the shape and structure of a ligand or substrate defined in relation to the molecule's spatial association with a binding pocket of the invention. Generally, a method is provided for designing potential inhibitors of an F-box protein-substrate interaction or SCF E3 ubiquitin ligase-substrate interaction comprising the step of applying the structural coordinates of a substrate or ligand defined in relation to its spatial association with a binding pocket, or a part thereof, to generate a compound that is capable of associating with the binding pocket.

It will be appreciated that a modulator of an F-box protein or SCF E3 ubiquitin ligase may be identified by generating an actual secondary or three-dimensional model of a binding pocket, synthesizing a compound, and examining the components to find whether the required interaction occurs.

30 A potential modulator of an F-box protein or SCF E3 ubiquitin ligase identified by a method of the present invention may be confirmed as a modulator by synthesizing the compound, and testing its effect on the F-box protein or SCF E3 ubiquitin ligase in an assay.

35 A modulator of the invention may be converted using customary methods into pharmaceutical compositions. A modulator may be formulated into a pharmaceutical composition containing a modulator either alone or together with other active substances.

Therefore, the methods of the invention for identifying modulators may comprise one or more of the following additional steps:

- (a) testing whether the modulator is a modulator of the activity of an F-box protein or an SCF E3 ubiquitin ligase, preferably testing the activity of the modulator in cellular assays and animal model assays;
- (b) modifying the modulator;
- (c) optionally rerunning steps (a) or (b); and
- (d) preparing a pharmaceutical composition comprising the modulator.

Steps (a), (b) (c) and (d) may be carried out in any order, at different points in time, and they need not be sequential.

Still another aspect of the present invention provides a method of conducting a drug discovery business comprising:

- (a) providing one or more systems employing the atomic interactions, atomic contacts, or structural coordinates of a binding pocket of an F-box protein or SCF E3 ubiquitin ligase involved in substrate recognition and/or orientation, for identifying agents by their ability to inhibit or potentiate the atomic interactions or atomic contacts of a binding pocket;
- (b) conducting therapeutic profiling of agents identified in step (a), or further analogs thereof, for efficacy and toxicity in animals; and
- (c) formulating a pharmaceutical preparation including one or more agents identified in step (b) as having an acceptable therapeutic profile.

A further aspect of the present invention provides a method of conducting a drug discovery business comprising:

- (a) providing one or more systems for identifying agents by their ability to inhibit or potentiate the interaction between an F-box protein or SCF complex and its substrate; and
- (b) conducting therapeutic profiling of agents identified in step (a), or further analogs thereof, for efficacy and toxicity in animals; and
- (c) formulating a pharmaceutical preparation including one or more agents identified in step (b) as having an acceptable therapeutic profile.

In certain embodiments, the subject methods can also include a step of establishing a distribution system for distributing the pharmaceutical preparation for sale, and may optionally include establishing a sales group for marketing the pharmaceutical preparation.

Yet another aspect of the invention provides a method of conducting a target discovery business comprising:

- (a) providing one or more systems employing the atomic interactions, atomic contacts, or structural coordinates of a binding pocket of an F-box protein or SCF complex involved in substrate

recognition and/or orientation, for identifying agents by their ability to inhibit or potentiate the atomic interactions or atomic contacts;

- (b) (optionally) conducting therapeutic profiling of agents identified in step (a) for efficacy and toxicity in animals; and
- (c) licensing, to a third party, the rights for further drug development and/or sales for agents identified in step (a), or analogs thereof.

Methods are also provided for regulating an F-box protein – substrate interaction or an SCF E3 ubiquitin ligase–substrate interaction by changing a binding pocket involved in substrate recognition and/or orientation. A binding pocket may be changed by altering amino acid residues forming the binding pocket (e.g. introducing mutations) or using a modulator.

The invention also contemplates a method of treating or preventing a condition or disease associated with an F-box protein or an SCF E3 ubiquitin ligase in a cellular organism, comprising:

- (a) administering a modulator of the invention in an acceptable pharmaceutical preparation; and
- (b) potentiating or inhibiting the F-box protein or SCF E3 ubiquitin ligase to treat or prevent the disease.

In an embodiment the condition or disease is cancer or Alzheimer's disease.

The invention provides for the use of a modulator identified by the methods of the invention in the preparation of a medicament to treat or prevent a disease in a cellular organism. Use of modulators of the invention to manufacture a medicament is also provided.

These and other aspects of the present invention will become evident upon reference to the following detailed description and Tables, and attached drawings.

DESCRIPTION OF THE DRAWINGS AND TABLES

The present invention will now be described only by way of example, in which reference will be made to the following Figures:

Figure 1 shows structure based sequence alignments of (A) Skp1 orthologs and (B) Cdc4 orthologs (red) and paralogs (black). Human Fbw7 and β -TrCP1 are isoforms 1 and 2, respectively. Secondary structure elements are colored as in Figure 2A. Disordered regions in the crystal structure are shown as dashed lines. Red residues are essential for the Cdc4 function, blue residues strongly influence but do not abrogate function, green residues are non-essential but conserved around the binding pocket, and yellow residues are conserved elsewhere. Circles indicate mutations associated with excessive cell proliferation in flies and/or cancer in humans. Deletion of residues 37-64 in Skp1 is denoted by a triangle and a replacement of two closely placed loops from residues 602-605 and 609-624 is denoted by the underline of the short interloop sequence Gly-Glu-Leu. Insertions to optimize sequence alignments are indicated by number of residues inserted in gray. The non-standard β -strand element 9¹ in ScCdc4 is marked by the red asterisk and is shown in full at the bottom of the alignment. Residues that anchor helix α 6 to the F-box domain are

marked by green hearts, those that anchor helix $\alpha 6$ to the WD40 domain by red hearts and those that make direct contact between the WD40 domain and F-box domain by blue asterisks. [SEQ ID NOs 3-16.]

Figure 2 shows an overview of the Skp1-Cdc4-CPD complex. (A) Ribbon representation of Skp1 and the F-box domain (274-319), the helical linker region (331-366), and the WD40 domain of Cdc4 (367-744) coloured green, red, pink, and blue, respectively. The bound cyclin E derived CPD peptide is shown in purple with the phosphothreonine moiety shown in ball and stick representation. Secondary structure elements are indicated. Positions of disordered loop regions are shown as ribbon breaks. All ribbons representations were generated using Ribbons. (B) Ribbons representation highlighting the WD 40 domain of Cdc4. β propeller blades are denoted PB1 to PB8, and the component secondary structure elements are indicated. Ribbons and CPD peptide are coloured as in (A). Position of the WD40 domain is identical to that in Figures 4A to 4C. (C) The structured linkage between the WD40 domain and the F box domain of Cdc4.

Figure 3 shows an overview of the CPD binding region of the Cdc4 WD40 repeat domain. (A) Molecular surface representation of the CPD binding pocket indicating invariant and highly conserved residues. Basic, hydrophobic and small residues are coloured blue, green and orange respectively. The bound CPD is shown in ball and stick representation with carbon, nitrogen, oxygen and phosphorous atoms coloured white, blue, red and yellow respectively. All surface representation were generated using Grasp. (B) Surface representation of CPD binding region as oriented in (A) coloured according to electrostatic potential. Blue and red indicate regions of positive and negative potential respectively (10 to -10 k_BT). Residues of the bound CPD are labeled. (C) Stereo ribbons representation highlighting side chains and molecular interactions in the CPD binding pocket. CPD residues and highly conserved and invariant Cdc4 residues are displayed in ball and stick representation. Sites of mutation that give rise to severe loss of function are coloured red, and intermediate loss of function are coloured yellow (see Table 5). All other highly conserved and invariant residues are coloured green. Reference propeller blades of the WD40 repeat domain are indicated. (D) Stereo ribbons representation of the CPD binding pocket highlighting cancer causing mutations in drosophila and human Cdc4 orthologues. Arginine mutations in H-cell lines or endometrial cells are coloured red. Drosophila mutations are coloured blue and Cdc4 temperature sensitive mutations (Rosamond personal communication) are coloured yellow. (E) Multiple Anomalous Dispersion phased electron density map corresponding to the CPD bound to the WD40 repeat domain of Cdc4. Refined CPD model is shown in ball and stick representation. Figure generate using O. (F) Schematic of CPD binding pocket interactions with the CPD peptide.

Figure 4 shows (A) Stereo ribbons representation of the human Skp1-Skp2 complex superimposed on the yeast Skp1-Cdc4-CPD complex. Human Skp1-Skp2 and yeast Skp1-Cdc4 were superimposed through a least squares optimization of Skp1 β strands 1 to 3 and α -helices 1 to 6 (RMSD = 0.74Å). The yeast Skp1-Cdc4 complex is coloured as in Figure 2. Human Skp1, the Skp2 F-box, and the Skp2 Leucine-rich repeat domain are coloured orange, green, and light blue, respectively. Skp1 and F box secondary structure elements that deviate significantly in size and position between the two structures are labeled. (B) Model of the SCF^{Cdc4-CPD} E2 complex. The yeast Skp1-Cdc4-CPD complex is coloured as in Figure 2. Cull1, Rbx1, and E2 proteins are coloured pink, red, and light blue, respectively.

The arrow indicates the distance between the peptide binding site and the active site cysteine of the E2. The structure was generated using the ternary complex of the cullin cdc53, rbx1, Skp1, previously reported, and superimposing the E2 structure from the E2/Cbl ring finger structure and the structure of Skp1, Cdc4 and a phosphorylated CPD peptide

Figure 5 shows (A) Selection of Sic1 phosphoisoforms by wild type and mutant forms of Cdc4. (B) In vitro ubiquitination of Sic1 isoforms by wild type and mutant SCFCdc4 complexes. (C) Natural CPD sites deviate from the optimal CPD by one or more or more residues.

Figure 6 shows substrate orientation within the Skp1-Cdc4-CPD complex. (A) Comparison of the ScSkp1-ScCdc4-CPD complex and the hSkp1-hSkp2 complex. Complexes were superimposed through a least squares optimization of Skp1 β -strands 1 to 3 and α -helices 1 to 6 (RMSD C α = 0.74Å). Skp1 and F-box secondary structure elements that deviate significantly in size and position between the two structures are labeled. (B) Model of the ubiquitin-E2-SCF^{Cdc4}-CPD complex. The arrow indicates the 59Å distance separating the phosphate group of the CPD and the active site cysteine of the E2.

Figure 7 shows the CPD binding pocket of the WD40 domain. (A) Surface representation of the CPD binding pocket indicating invariant and highly conserved residues. Basic (blue), hydrophobic (green) and small polar residues (orange) are shown. The bound CPD is in ball and stick representation with carbon (white), nitrogen (blue), oxygen (red) and phosphorous (yellow) atoms shown. (B) Surface representation of CPD binding region indicating electrostatic potential. Blue and red indicate regions of positive and negative potential, respectively, over the range 10 to -10 k_BT. (C) Stereo ribbons representation of side chains and molecular interactions in the CPD binding pocket. Highly conserved and invariant side chains of Cdc4 and the CPD are displayed in ball and stick representation. Sites of mutation that give rise to severe and intermediate loss of function (see Figure 8) are colored red and blue, respectively; non-essential residues are colored green.

(D) Schematic of CPD binding pocket interactions with the CPD peptide.

Figure 8 shows structure-guided mutational analysis of Cdc4. (A) Residues required for interaction of phospho-Sic1 and Cdc4 in vitro. Sic1 was phosphorylated with Cln2-Cdc28 kinase and captured onto resin loaded with either wild type or the indicated mutant forms of Skp1-Cdc4 complex. (B) Residues essential for Cdc4 function in vivo. Complementation of a *cdc4Δ* strain by the indicated alleles was assessed in a plasmid shuffle assay. The R485A, R467A and R534A mutations in Cdc4 have been previously shown to disrupt function in vivo (Nash et al., 2001) and so are not shown. (C) Effect of Cdc4 mutations on sensitivity to increased *SIC1* dosage. Strains bearing indicated *CDC4* alleles were tested for sensitivity to overexpression of wild type *SIC1* and a partially stabilized version, *SIC1*^{Thr33Val} from the *GAL1* promoter. Strains were incubated on galactose or glucose medium for 2 days at 30°C.

Figure 9 shows the modulation of the multisite requirement for phospho-Sic1-Cdc4 interaction. (A) All natural CPD sites in Sic1 deviate from the CPD consensus. Underlined residues indicate sub-optimal residues at the P-1 and P-2 positions, boxed residues indicate sub-optimal basic residues at the P+2 to P+5 positions and asterisks indicate a sub-optimal pSer at the P0 position. (B) Capture of Sic1 phospho-isoforms by wild type and mutant Cdc4.

Pools of differentially phosphorylated Sic1 were captured on Skp1–Cdc4 resin, using either wild type or the indicated mutant forms of Cdc4 compromised for selection at the P-1 position (V384N W717N) or the P+2 to P+5 positions (K402A R443D). The input and bound phospho-Sic1 isoform pools were resolved by denaturing IEF-2D gel electrophoresis and visualized by anti-Sic1 immunoblot. (C) Ubiquitination of phospho-Sic1 isoforms by wild type and mutant SCF^{Cdc4} complexes. Pools of differently phosphorylated Sic1 were incubated in solution with an equimolar amount of the indicated SCF^{Cdc4} complexes, Cdc34, ubiquitin and ATP for 1 h at 30°C. Input and reaction products were separated and visualized as in (B). Arrows indicate the less phosphorylated forms of Sic1 captured by Cdc4 selection mutants. Asterisk indicates more extensively ubiquitinated species (D) Possible interaction mechanisms for single site and multi-site dependent substrate binding to Cdc4. In a two-site cooperative interaction model (left), a primary high affinity CPD binding site acts in conjunction with a secondary weak CPD binding site. The free energy for the two interactions is additive and so the overall K_d increases multiplicatively. In a single-site allovalent interaction (right), multiple low affinity CPD sites engage a single CPD binding site on Cdc4 in equilibrium. The high local concentration of CPD sites increases the probability of binding such that Sic1 is unable to diffuse away from Cdc4 before re-binding occurs. The probability of re-binding increases as an exponential function of the number of CPD sites, thus accounting for the apparent cooperativity of the interaction.

The present invention will now be described only by way of example, in which reference will be made to the following Tables:

Table 1 shows data collection, structure determination and refinement statistics of a crystal of the invention.

Table 2 shows data collection, structure determination and refinement statistics of a crystal of the invention.

Table 3 shows intermolecular contacts in a binding pocket of the invention.

Table 4 shows intermolecular contacts in a binding pocket of the invention.

Table 5 shows mutant cdc4 polypeptides of the invention. Mutational analysis of the CPD binding surface. Mutants were tested *in vitro* by ability to bind phosphorylated Sic1 and then captured onto GST-Skp1/Cdc4 resin and detected with anti-sic1 antibody. Mutants were tested *in vivo* by ability to degrade GAL1-SIC1 or various phosphorylation mutants. Sites are as follows: 3 = Thr 33, Thr 45, Ser 76; 4 = Thr 5, Thr 33, Thr 45, Ser 76; 5 = Thr 2, Thr 5, Thr 33, Thr 45, Ser 76; 6 = Thr 2, Thr 5, Thr 33, Thr 45, Ser 69, Ser 76; 7 = Thr 2, Thr 5, Thr 33, Thr 45, Ser 69, Ser 76, Ser 80. GAL1-SIC1 plasmids were transformed into a cdc4Δ strain containing a copy of CDC4 on a TRP1 ARS CEN plasmid. Strains were incubated for 2 days at 30°C.

Table 6 shows the structural coordinates of a binding pocket of the invention.

In Table 6, from the left, the second column identifies the atom number; the third identifies the atom type; the fourth identifies the amino acid type; the sixth identifies the residue number; the seventh identifies the x coordinates; the eighth identifies the y coordinates; the ninth identifies the z coordinates; the tenth identifies the occupancy; and the eleventh identifies the temperature factor.

Table 7 lists the oligonucleotides used in the studies described in the examples.

Table 8 lists the plasmids used in the studies described in the examples.

DETAILED DESCRIPTION OF THE INVENTION

In accordance with the present invention there may be employed conventional molecular biology, microbiology, and recombinant DNA techniques within the skill of the art. Such techniques are explained fully in the literature. See for example, Sambrook, Fritsch, & Maniatis, *Molecular Cloning: A Laboratory Manual*, Second Edition (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, N.Y); DNA Cloning: A Practical Approach, Volumes I and II (D.N. Glover ed. 1985); *Oligonucleotide Synthesis* (M.J. Gait ed. 1984); *Nucleic Acid Hybridization* B.D. Hames & S.J. Higgins eds. (1985); *Transcription and Translation* B.D. Hames & S.J. Higgins eds (1984); *Animal Cell Culture* R.I. Freshney, ed. (1986); *Immobilized Cells and enzymes* IRL Press, (1986); and B. Perbal, *A Practical Guide to Molecular Cloning* (1984).

GLOSSARY

Abbreviations for amino acid residues are the standard 3-letter and/or 1-letter codes used in the art to refer to one of the 20 common L-amino acids. Likewise abbreviations for nucleic acids are the standard codes used in the art.

“ Skp1-Cdc53/Cullin-F-box protein (SCF) E3 ubiquitin ligases” or “SCF complex” refers to a protein complex comprising the adaptor protein Skp1, the scaffold protein cdc53/cullin, a RING-H2 domain protein Rbx1 (also called Roc1 or Hrt1), and an F-box protein, which protein complex augments or otherwise facilitates the ubiquitination of a protein. In certain aspects of the present invention an SCF complex refers to a complex comprising Skp1 and an F box protein or parts thereof.

In the context of the present invention the term “F-box protein” refers to a protein comprising a characteristic structural motif called the F-box as described in Bai et al, (1996 *Cell* 86: 263-274) and a protein-protein interaction domain, in particular a WD40 repeat motif or domain. Examples of F-box Proteins include Cdc4 polypeptides, and homologs or portions thereof, preferably portions that interact with a CPD motif (e.g. WD repeat).

A “WD40 repeat”, “WD40 motif”, or “WD repeat domain” is generally defined as a contiguous sequence of about 25 to 50 amino acids with relatively-well conserved sets of amino acids [i.e. Trp-Asp (WD)] at the ends (amino- and carboxyl- terminal) of the sequence. (For reviews see Neer EJ, Schmidt CJ, Nambudripad R & Smith TF: “The ancient regulatory-protein family of WD-repeat proteins,” *Nature* 371, 297-300 (1994) PMID: 8090199; and Smith TF, Gaitatzes CG, Saxena K & Neer EJ: “The WD-repeat: a common architecture for diverse functions,” *TIBS* 24, 181-185 (1999) PMID: 10322433.) A WD repeat motif or domain can also be defined as a domain of an F-box protein that interacts with a CPD motif or like motif.

Examples of WD-repeat-containing proteins are cdc4 polypeptides, Met30 homologues and orthologues (see for example, GenBank Accession No. P39014 or MT30_YEAST - SEQ ID NO.17) and β -TRCP homologues and orthologues (see for example, GenBank Accession No. NP_033901 - SEQ ID NO.18). Other WD40 repeat-containing proteins will, however, be appreciated by those skilled in the art. A WD40-repeat protein also includes a part of the protein. A person skilled in the art may conduct searches to identify proteins that contain WD-40 repeats, in particular F-box proteins. For example, on-line databases such as GenBank or SwissProt can be searched, either with an entire sequence of a WD-40-containing protein, or with a consensus WD-40 repeat sequence. Various search algorithms

and/or programs may be used, including FASTA, BLAST or ENTREZ. FASTA and BLAST are available as a part of the GCG sequence analysis package (University of Wisconsin, Madison, Wis.). ENTREZ is available through the National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, Md. The number of WD-40 repeats in a particular protein can range from two to more than eight.

5 A "Cdc4 Phospho-Degron motif" or "CPD motif" is a motif that targets substrates for ubiquitination by SCF complexes. The motif can be defined by the consensus sequence X²-X³-pThr-Pro-X⁴ (SEQ ID NO.19), more particularly X²-X³-pThr-Pro-X⁴-X⁵-X⁶-X⁷ (SEQ ID NO.20), wherein X² represents Leu, Pro, or Ile, preferably Leu or Ile; X³ represents Leu, Ile, Val, or Pro, preferably Ile, Leu, or Pro; X⁴ represents any amino acid except basic and bulky hydrophobic amino acids, preferably X⁴, X⁵ and X⁶ represent any amino acid except basic and bulky hydrophobic amino acids, preferably X⁴ is any amino acid except Arg, Lys, Tyr, or Trp, more preferably X⁴ is Ile, Val, Pro, or Gln, preferably X⁵ and X⁶ are any amino acid except Arg, Lys, or Tyr and more preferably X⁵ is Gln, Leu, Met, Thr, or Glu, and X⁶ is Gln, Ala, Thr, Glu, or Ser; and X⁷ is any amino acid, preferably not a basic or bulky hydrophobic amino acid, more preferably X⁷ is any amino acid except Arg, Lys, or Tyr, most preferably X⁷ is Leu, Trp, Asp, Pro, or Gly. A CPD motif preferably comprises the consensus sequence -Leu/Gly/Tyr-Pro-pThr-Pro- (SEQ ID NO.21).

15 A CPD motif containing protein includes proteins comprising the CPD motif including but not limited to Gcn4, Cyclin E, Far1, Ash1, Sic1, Pc17, Cdc16, p27^{kip1}, Cln2, and transcription factors such as β catenin or $\text{I}\kappa\text{B}\alpha$, and homologues of these proteins. The term includes but is not limited to all homologs, orthologs, naturally occurring allelic variants, isoforms and precursors of the polypeptides. Other proteins containing CPD motif sequences may be identified with a protein homology search, for example by searching available databases such as GenBank or SwissProt and various search algorithms and/or programs may be used including FASTA, BLAST (available as a part of the GCG sequence analysis package, University of Wisconsin, Madison, Wis.), or ENTREZ (National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, Bethesda, MD).

20 The term "substrate" refers to a protein that interacts with an F-box protein targeting it for ubiquitin-dependent proteolysis, or a protein targeted for F-box dependent degradation. Examples of substrates are CPD motif containing proteins including Gcn4, CyclinE, Far1, Ash1, Sic1, Pc17, Cdc16, p27^{kip1}; Cln2, and, transcription factors such as β catenin or $\text{I}\kappa\text{B}\alpha$. The term also refers to a part of a protein that interacts with an F-box protein, including a CPD motif, and analogues of substrates or parts thereof

25 A "ligand" refers to a compound or entity that associates with a binding pocket, or modulators of an F-box protein or SCF E3 ubiquitin ligase, including inhibitors. A ligand may be designed rationally by using a model according to the present invention.

30 The terms "cdc4 polypeptide" is used to refer to polypeptides of the cdc4 family of proteins characterized by an F-box motif and WD repeats. The term includes but is not limited to all homologs, orthologs, naturally occurring allelic variants, isoforms and precursors of the polypeptides of GenBank Accession Nos. S56245 or SEQ ID NO. 22 (*Saccharomyces cerevisiae* cdc4), CAA65538 or SEQ ID NO. 23 (*Candida albicans* cdc4), AAL07271 or SEQ ID

NO. 24 (human cdc4), AAC47809 or SEQ ID NO. 25 (sel-10), AAK57547 or SEQ ID NO. 26 (*Homo sapiens* F-box protein FBW7), and AAG09623F or SEQ ID NO. 27 (*Homo sapiens* F box protein FBX30). In general, for example, naturally occurring allelic variants will share significant homology (70-90%) to these sequences. Allelic variants may contain conservative amino acid substitutions from cdc4 sequences or will contain a substitution of an amino acid from a corresponding position in a cdc4 homologue such as, for example, the human homologue. [See Strohmaier, H., Nature 413 (6853), 316-322 (2001) for a description and sequence of human cdc4]. The term also includes the mutant cdc4 polypeptides described herein. Figure 1 shows a structure based sequence alignment of cdc4 orthologs and paralogs.

The term "cdc53" or "cdc53 polypeptide" is used interchangeably herein with the term "cullins" when referring to a vertebrate homolog of the yeast cdc53 protein. The term "cullin polypeptide" or "cullin protein", refers to a member of the cullins family, e.g., any one of cul-1, -2, -3, -4, -5, or -6. The term includes but is not limited to all homologs, naturally occurring allelic variants, isoforms and precursors of a cdc53 polypeptide or cullin of GenBank Accession Nos. AAB38821 or SEQ ID NO. 28 (*Saccharomyces cerevisiae* cdc53), AAC36304 or SEQ ID NO. 29 (*Homo sapiens* cullin 3), AAC51190 or SEQ ID NO. 30 (*Homo sapiens* cullin 2), NP_003581 or SEQ ID NO. 31 (*Homo sapiens* cullin 3), AF126404_1 or SEQ ID NO. 32 (*Homo sapiens* cullin 2), CUL1_CAEEL or SEQ ID NO. 33 (*Caenorhabditis elegans* cullin 1), AAA85085 or SEQ ID NO. 34 (*Drosophila melanogaster* cullin 1) and the cullins described in Kipreos ET (Cell 1996 Jun 14;85(6):829-39). In general for example, naturally occurring allelic variants of cdc53 will share significant homology (70-90%) to the cdc53 or cullin sequences. Allelic variants may contain conservative amino acid substitutions from the cdc4 sequence or will contain a substitution of an amino acid from a corresponding position in a cdc4 homolog such as, for example, the human homolog.

The term "Skp1" or "Skp1 polypeptide" is used to refer to polypeptides that connect cell cycle regulators to the ubiquitin proteolysis machinery by associating with F-box proteins through the F-box motif. The term includes but is not limited to all homologs, naturally occurring allelic variants, isoforms and precursors of Skp1 of GenBank Accession Nos. SKP1_SCHPO or SEQ ID NO. 35 (*Schizosaccharomyces pombe*), BAB62325 or SEQ ID NO. 36 (*Schizosaccharomyces pombe*), AAC49492 or SEQ ID NO. 37 (*Saccharomyces cerevisiae*), and AAB17500 or SEQ ID NO. 38 (*Saccharomyces cerevisiae*). In general, for example, naturally occurring allelic variants of Skp1 will share significant homology (70-90%) to the Skp1 sequences. Allelic variants may contain conservative amino acid substitutions from the Skp1 sequence or will contain a substitution of an amino acid from a corresponding position in a Skp1 homolog such as, for example, the human homolog. Figure 1 shows a structure based sequence alignment of Skp1 homologues.

A CPD motif and WD repeat or proteins containing same, cdc4 polypeptides, cdc53, Skp1, substrates, and SCF complexes, may be from any species, particularly a mammalian species, including bovine, ovine, porcine, murine, equine, preferably the human species, and from any source, whether natural, synthetic, semi-synthetic, or recombinant.

The term "agonist" of a binding pocket refers to a compound or ligand that interacts with the binding pocket and maintains or increases the activity of the binding pocket to which it binds. The term includes partial agonists and inverse agonists. Agonists may include proteins, peptides, nucleic acids, carbohydrates, or any other molecules that bind to a binding pocket. Agonists also include a molecule derived from a binding pocket. Peptide mimetics, synthetic molecules with physical structures designed to mimic structural features of particular peptides, may serve as agonists. The stimulation may be direct, or indirect, or by a competitive or non-competitive mechanism. The term includes partial agonists and inverse agonists.

As used herein, the term "partial agonist" means an agonist that is unable to evoke the maximal response of a biological system, even at a concentration sufficient to saturate the specific receptors.

As used herein, the term "partial inverse agonist" is an inverse agonist that evokes a submaximal response to a biological system, even at a concentration sufficient to saturate the specific receptors. At high concentrations, it will diminish the actions of a full inverse agonist.

The term "antagonist", as used herein, refers to a ligand or compound that binds a binding pocket but does not maintain the activity of the binding pocket to which it binds. The term can also include a ligand that reduces the action of another agent, such as an agonist. An antagonistic action may result from a combination of the substance being antagonised (chemical antagonism) or the production of an opposite effect through a different protein (functional antagonism or physiological antagonism) or as a consequence of competition for the binding site of an intermediate that links a protein to the effect observed (indirect antagonism). The antagonist may act at the same site as the agonist (competitive antagonism). Antagonists may include proteins, peptides, nucleic acids, carbohydrates, or any other molecules that bind to a binding pocket. Antagonists also include a molecule derived from a binding pocket. Peptide mimetics, synthetic molecules with physical structures designed to mimic structural features of particular peptides, may serve

As used herein, the term "competitive antagonism" refers to the competition between an agonist and an antagonist for a binding pocket of a protein that occurs when the binding of agonist and antagonist becomes mutually exclusive. This may be because the agonist and antagonist compete for the same binding sites or pockets, or combine with adjacent but overlapping sites. A third possibility is that different sites are involved but that they influence the receptor macromolecules in such a way that agonist and antagonist molecules cannot be bound at the same time. If the agonist and antagonist form only short lived combinations with a binding pocket so that equilibrium between agonist, antagonist and binding pocket is reached during the presence of the agonist, the antagonism will be surmountable over a wide range of concentrations. In contrast, some antagonists, when in close enough proximity to their binding site, may form a stable covalent bond with it and the antagonism becomes insurmountable when no spare receptors remain.

By being "derived from" a binding pocket is meant any molecular entity which is identical or substantially equivalent to the binding pocket. A peptide derived from a binding pocket may encompass the amino acid sequence of a naturally occurring binding pocket, any portion of that binding pocket or other molecular entity that functions to

bind to an associated or interacting binding pocket. A peptide derived from such a binding pocket will interact directly or indirectly with an associated molecule in such a way as to mimic the native binding pocket. Such peptides may include competitive inhibitors, peptide mimetics, and the like. The entity will not include a full length sequence of a wild-type molecule. Peptide mimetics, synthetic molecules with physical structures designed to mimic structural features of particular peptides, may serve as inhibitors or enhancers.

“Peptide mimetics” are structures which serve as substitutes for peptides in interactions between molecules (See Morgan et al (1989), *Ann. Reports Med. Chem.* 24:243-252 for a review). Peptide mimetics include synthetic structures which may or may not contain amino acids and/or peptide bonds but retain the structural and functional features of a peptide, or agonist or antagonist (i.e. enhancer or inhibitor) of a binding pocket. Peptide mimetics also include peptoids, oligopeptoids (Simon et al (1972) *Proc. Natl. Acad. Sci USA* 89:9367); and peptide libraries containing peptides of a designed length representing all possible sequences of amino acids corresponding to a motif, peptide, or agonist or antagonist (i.e. enhancer or inhibitor) of the invention.

Sequences are “homologous” or considered “homologs” when at least about 70% (preferably at least about 80 to 90%, and most preferably at least 95%) of the nucleotides or amino acids match over a defined length of the molecule. “Substantially homologous” also includes sequences showing identity to the specified sequence. Percent identity can be determined electronically, e.g., by using the MEGALIGN program (DNASTAR, Inc., Madison Wis.) which can create alignments between two or more sequences according to different methods, e.g., the clustal method. (See, e.g., Higgins, D. G. and P. M. Sharp (1988) *Gene* 73:237-244.) Percent identity can also be determined by other methods known in the art, (e.g., the Jotun Hein method. (See, e.g., Hein, J. (1990) *Methods Enzymol.* 183:626-645) or by varying hybridization conditions). Preferably, the amino acid or nucleic acid sequences have an alignment score of greater than 5 (in standard deviation units) using the program ALIGN with the mutation gap matrix and a gap penalty of 6 or greater (Dayhoff).

BINDING POCKET

“Binding pocket” refers to a region or site of an F-box protein or molecular complex thereof (e.g. Skp1-F-box complex, SCF E3 ubiquitin ligase) involved in substrate selection and/or orientation. As the result of its shape, a binding pocket associates with another region of an F-box protein or SCF complex or with a substrate or a part thereof.

In an aspect of the invention a binding pocket comprises one or more of the residues involved in selection and/or orientation of a substrate or ligand.

In an aspect of the invention a binding pocket is provided that comprises the WD40 repeat domain of an F-box protein. In another embodiment the binding pocket comprises a WD40 repeat domain and a helical linker of an F-box protein. In a further embodiment, the binding pocket comprises a WD40 repeat domain, a helical linker and an F-box domain of an F-box protein. In an embodiment the F-box protein is a cdc4 polypeptide or portion thereof.

A binding pocket of the invention may comprise a WD40 repeat domain characterized by one or more of the following characteristics:

- (a) a 7 or 8 blade β -propeller structure, in particular a 8 blade β -propeller structure;
- (b) a disk like structure characterized by a cavity in the middle and two opposing circular surfaces of different size;
- (c) a conical frustum of about 40Å top surface and about 50Å bottom surface, an overall thickness of 30Å and a central pore of 6Å diameter; and
- (d) a CPD binding site on the top surface of the frustum of (c) and running across the edge of the pore, while the bottom surface of the frustum links to the F-box domain.

A binding pocket of the invention may be characterized by one or more of the following characteristics:

- (i) a dedicated pThr-Pro binding pocket;
- (ii) a deep hydrophobic pocket that selects hydrophobic residues N-terminal to the phosphorylation site of a CPD, and
- (iii) a through space electrostatic selection against basic residues C-terminal to the phosphorylation site of a CPD.

A binding pocket of the invention may comprise a helical linker characterized by α helices that form a stalk and pedestal like structure that connects and orients a WD repeat domain. The helical linker binding pocket can also be characterized by one or more of the following:

- (a) a helix (e.g. $\alpha 6$ in Figure 2 or Figure 6) that is 30Å in length and is anchored at its N-terminus to the hydrophobic core of the F-box/helical extension and at its C-terminus to the hydrophobic core of a WD repeat domain,
- (b) the helix of (a) (e.g. $\alpha 6$) anchored at its amino terminus to an F-box through hydrophobic interactions (e.g. involving $\alpha 6$ residues Phe 355, Leu356, and F box residues Ile295, Ile296, Leu315, Leu 319 and Trp316 of Cdc4 or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (c) a second helix (e.g. helix 5) packed along the base of the helix of (a) or (b) opposite to the F-box domain through hydrophobic interactions (e.g. involving Tyr342, Leu338, and Leu 334 of Cdc4 or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (d) the helix of (a) (e.g. helix $\alpha 6$) anchored at its C-terminus through hydrophobic interactions;
- (e) a C-terminal end of helix $\alpha 6$ inserted obliquely between propeller blades $\beta 7$ and $\beta 8$ of a WD40 domain through van der Waals and hydrophobic interactions (e.g. involving Trp365 and Ile361 with WD40 domain residues Val687, Ile696, Leu726, and Phe743 in β -propeller blades 7 and 8 of Cdc4 or the corresponding residues in Cdc4 homologs, variants, precursors etc.).

A CPD motif binding pocket of the invention may comprise a hydrophobic pocket that surrounds the open central channel of a 7 or 8 blade WD repeat propeller. A binding pocket of Cdc4 is more particularly characterized by one or more of the following:

- (a) a WD repeat domain surface composed of invariant and highly conserved residues from β -propeller blades;
- (b) a three-sided pocket formed by Trp426, Thr386, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- 5 (c) a three-sided pocket formed by Trp426, Thr441, Thr 465, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (d) a hydrophobic pocket composed of Trp 426, Trp 717, Thr 386, and Val 384 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (e) a pocket formed by Leu634, Met590, and Tyr574 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.); and
- 10 (f) a pocket formed by Arg485, Arg467, Arg534, Tyr548, and Arg572 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);.

A binding pocket may comprise one or more of the amino acid residues for an F-box protein crystal or F-box protein –substrate crystal identified in Table 3 or Table 4. In an aspect the binding pocket comprises the atomic contacts of atomic interactions 1 to 4 or interactions 5 to 8/9 identified in Table 3 or Table 4. In an aspect of the invention the binding pocket comprises all of the amino acid residues identified in Table 3 or Table 4.

The term "binding pocket" (BP) also includes a homolog of the binding pocket or a portion thereof. As used herein, the term "homolog" in reference to a binding pocket refers to a binding pocket or a portion thereof which may have deletions, insertions or substitutions of amino acid residues as long as the binding specificity is retained. In this regard, deliberate amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues as long as the binding specificity of the binding pocket is retained.

As used herein, the term "portion thereof" means the structural coordinates corresponding to a sufficient number of amino acid residues of a binding pocket (or homologs thereof) that are capable of associating with a substrate (e.g. CPD motif) or ligand. For example, the structural coordinates provided in a crystal structure may contain a subset of the amino acid residues in a binding pocket which may be useful in the modelling and design of compounds that bind to the binding pocket.

CRYSTAL

The invention provides crystal structures. As used herein, the term "crystal" or "crystalline" means a structure (such as a three dimensional (3D) solid aggregate) in which the plane faces intersect at definite angles and in which there is a regular structure (such as internal structure) of the constituent chemical species. The term "crystal" can include any one of: a solid physical crystal form such as an experimentally prepared crystal, a crystal structure derivable from the crystal (including secondary and/or tertiary and/or quaternary structural elements), a 2D and/or 3D model based on the crystal structure, a representation thereof such as a schematic representation thereof or a diagrammatic representation thereof, or a data set thereof for a computer.

In one aspect, the crystal is usable in X-ray crystallography techniques. Here, the crystals used can withstand exposure to X-ray beams used to produce a diffraction pattern data necessary to solve the X-ray crystallographic structure. A crystal may be characterized as being capable of diffracting x-rays in a pattern defined by one of the crystal forms depicted in Blundel et al 1976, Protein Crystallography, Academic Press.

5 A crystal of the invention is generally produced in a laboratory; that is, it is an isolated crystal produced by an individual.

The invention contemplates a crystal comprising a binding pocket of the invention, in particular a binding pocket of an F-box protein or SCF complex or portion thereof, involved in substrate selection and/or orientation.

10 In an aspect of the invention a crystal is provided that comprises the WD40 repeat domain of an F-box protein, in particular Cdc4. In another embodiment the crystal comprises a WD40 repeat domain and a helical linker of an F-box protein. In a further embodiment, the crystal comprises a WD40 repeat domain, a helical linker and an F-box domain of an F-box protein. In an embodiment the F-box protein is a cdc4 polypeptide or portion thereof.

A crystal of the invention comprising a WD40 repeat domain, in particular a Cdc4 polypeptide WD40 repeat domain, may be characterized by one or more of the following characteristics:

- 15 (a) a 7 or 8 blade β -propeller structure, in particular a 8 blade β -propeller structure;
- (b) a disk like structure characterized by a cavity in the middle and two opposing circular surfaces of different size;
- (c) a conical frustum of about 40Å top surface and about 50Å bottom surface, an overall thickness of 30Å and a central pore of 6Å diameter; and
- 20 (d) a CPD binding site on the top surface of the frustum of (c) and running across the edge of the pore, while the bottom surface of the frustum links to the F-box domain.

Each blade of the β -propeller structure can be further characterized by 4 anti-parallel β -strands. The disk like structure can also be characterized by a smaller surface comprising a CPD binding site and a bottom surface anchored by a helix (e.g. helix α 6) of a helical extension of the F-box protein. As illustrated in Figures 2 and 3 the structure is further characterized by β -propeller blade 2 consisting of 5 β -strands and a strand β 9' forming a parallel arrangement with strand β 9.

A crystal of a binding pocket of an F-box protein of the invention, in particular a Cdc4 polypeptide, may be characterized by one or more of the following characteristics:

- 30 (i) a dedicated pThr-Pro binding pocket;
- (ii) a deep hydrophobic pocket that selects hydrophobic residues N-terminal to the phosphorylation site of a CPD motif, and
- (iii) a through space electrostatic selection against basic residues C-terminal to the phosphorylation site of a CPD motif.

In a preferred embodiment, a crystal of a WD40 repeat domain has the structure illustrated in Figure 2 or 3.

A crystal of the invention can comprise a helical linker characterized by α helices that form a stalk and pedestal like structure that connects and orients a WD repeat domain. A helical linker structure of a Cdc4 polypeptide can also be characterized by one or more of the following structures:

- (a) a helix (e.g. $\alpha 6$ in Figure 2 or Figure 6) that is 30Å in length and is anchored at its N-terminus to the hydrophobic core of the F-box/helical extension and at its C-terminus to the hydrophobic core of a WD repeat domain,
- (b) the helix of (a) (e.g. $\alpha 6$) anchored at its amino terminus to an F-box through hydrophobic interactions (e.g. involving $\alpha 6$ residues Phe 355, Leu356, and F box residues Ile295, Ile296, Leu315, and Trp316 or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (c) a second helix (e.g. helix 5) packed along the base of the helix of (a) or (b) opposite to the F-box domain through hydrophobic interactions (e.g. involving Tyr342, Leu338, and Leu 334) (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (d) the helix of (a) (e.g. helix $\alpha 6$) anchored at its C-terminus through hydrophobic interactions;
- (e) a C-terminal end of helix $\alpha 6$ inserted obliquely between propeller blades $\beta 7$ and $\beta 8$ of the WD40 domain through van der Waals and hydrophobic interactions (e.g. involving Trp365 and Ile361 with WD40 domain residues Val687, Ile696, Leu726, and Phe743 in β -propeller blades 7 and 8 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.).

In a preferred embodiment, a crystal of a helical linker has the structure illustrated in Figure 2.

A crystal of the invention may comprise a CPD motif binding pocket that is characterized by a hydrophobic pocket that surrounds the open central channel of a 7 or 8 blade WD repeat propeller. A crystal of a Cdc4 polypeptide may be more particularly characterized by one or more of the following:

- (a) a WD repeat domain surface composed of invariant and highly conserved residues from β -propeller blades;
- (b) a three-sided pocket formed by Trp426, Thr386, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (c) a three-sided pocket formed by Trp426, Thr441, Thr 465, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (d) a hydrophobic pocket composed of Trp 426, Trp 717, Thr 386, and Val 384 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (e) a pocket formed by Leu634, Met590, and Tyr574 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.); and
- (f) a pocket formed by Arg485, Arg467, Arg534, Tyr548, and Arg572 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.).

In a preferred embodiment, a crystal of a CPD motif binding pocket has the structure illustrated in Figure 3,

In a further aspect of the invention a crystal is provided comprising an F-box domain comprising five α helices. In a preferred embodiment, a crystal of an F-box domain has the structure illustrated in Figure 2 or Figure 6.

A crystal of the invention may comprise an F-box protein characterized by one or more of the following:

- (a) an F-box domain consisting of five α helices;
- (b) a WD 40 repeat domain characterized by 7 or 8 copies of a WD40 repeat motif forming a 7 or 8 blade β -propeller structure; and
- (c) two α helices that together with two α helices of the F-box domain forming a stalk and pedestal like structure that connects and orients the WD40 domain.

With reference to a crystal of the present invention, residues in a binding pocket may be defined by their spatial proximity to a substrate or ligand in the crystal structure. For example, a binding pocket may be defined by its proximity to a substrate molecule, or modulator.

A crystal of the invention includes a binding pocket in association with one or more moieties, including heavy-metal atoms i.e. a derivative crystal, or one or more substrates or ligands i.e. a co-crystal.

The term “associate”, “association” or “associating” refers to a condition of proximity between a moiety (i.e. chemical entity or compound or portions or fragments thereof), and a binding pocket. The association may be non-covalent i.e. where the juxtaposition is energetically favored by for example, hydrogen-bonding, van der Waals, or electrostatic or hydrophobic interactions, or it may be covalent.

The term “heavy-metal atoms” refers to an atom that can be used to solve an x-ray crystallography phase problem, including but not limited to a transition element, a lanthanide metal, or an actinide metal. Lanthanide metals include elements with atomic numbers between 57 and 71, inclusive. Actinide metals include elements with atomic numbers between 89 and 103, inclusive.

Multiwavelength anomalous diffraction (MAD) phasing may be used to solve protein structures using selenomethionyl (SeMet) proteins. Therefore, a complex of the invention may comprise a crystalline binding pocket with selenium on the methionine residues of the protein.

A crystal may comprise a complex between a binding pocket and one or more substrates or ligands. In other words the binding pocket may be associated with one or more ligands or molecules in the crystal. The ligand may be any compound that is capable of stably and specifically associating with the binding pocket. A ligand may, for example, be a modulator or analogue thereof. Therefore, a crystal may comprise a binding pocket comprising two or more of the amino acid residues of an F-box protein structure as described herein, that are capable of associating with or coordinating a CPD motif as described herein.

In an embodiment, a crystal of the invention comprises a complex between a binding pocket, and a substrate or analogue thereof. Therefore, the present invention also provides a crystal comprising a binding pocket of an F-box protein or a SCF complex and a substrate or analogue thereof. A substrate may be for example, a CPD motif or CPD motif containing protein. An analog of a substrate is one which mimics the substrate molecule, binding in the binding pocket, but which is incapable (or has a significantly reduced capacity) to take part in SCF E3 ubiquitin ligase activity.

In an embodiment, a crystal comprising a WD repeat domain of a Cdc4 polypeptide and a CPD motif is provided, which is characterized by one or more of the following:

- (a) a WD 40 repeat domain characterized by 7 or 8 copies of a WD40 repeat motif forming a 7 or 8 blade β -propeller structure comprising β -propeller blades 1, 2, 3, 4, 5, 6, and 7, and optionally 8;
- (b) the CPD motif binds in an extended manner across β -propeller blade 2 with the N-terminus oriented toward the central cavity of the WD repeat domain and the C-terminus oriented towards the outer rim;
- (c) the CPD binding surface of the WD repeat domain is composed of invariant and highly conserved residues from β -propeller blades 1 to 6 and optionally 8;
- (d) a P0 phosphate pThr of the CPD motif forms direct electrostatic interactions with the guanidium groups of Arg 485, Arg 467, and Arg 534 and a direct hydrogen bond with the side chain of Tyr 548 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.);
- (e) P +1 proline side chains of the CPD motif project into a three-sided pocket on the CPD binding surface formed by the side chain of Trp 426 and Arg485 or Trp 426, Thr441, Thr465, and Arg 485 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.); and
- (f) P+1 leucine side chain of the CPD motif is oriented towards a hydrophobic pocket composed of residues Trp 426, Trp 717, Thr 386, and Val 384 (or the corresponding residues in Cdc4 homologs, variants, precursors etc.).

In a preferred embodiment, a crystal of a complex of a WD repeat domain and a CPD motif has the structure illustrated in Figure 2, 3, 4, 6, or 7.

A crystal or secondary or three-dimensional structure of a binding pocket of an F-box protein, may be specifically defined by one or more of the atomic contacts of the atomic interactions identified in Table 3 or Table 4. The atomic interactions in Table 3 or Table 4 are defined therein by an atomic contact (more preferably, a specific atom of an amino acid residue where indicated) on the F box protein, in particular on the WD40 repeat domain or helical linker, and an atomic contact (more preferably, a specific atom of an amino acid residue where indicated) on a substrate e.g. CPD motif, or an atomic contact (more preferably, a specific atom of an amino acid residue where indicated) on another region of the F-box protein (e.g. helical linker or F-box domain). In certain embodiments, a crystal of the invention comprises the atomic contacts of atomic interactions 1 to 8 identified in Table 3 or Table 4. In certain particular embodiments a crystal is provided comprising the atomic contacts of atomic interactions 1 to 4 or 5 to 8. Preferably, a crystal is defined by the atoms of the atomic contacts in the binding pocket having the structural coordinates for the atoms listed in Table 6.

A structure of a complex may be defined by selected intermolecular contacts, preferably the structural coordinates of the intermolecular contacts as defined in Table 6, preferably interactions 5 to 8.

A crystal of the invention may comprise one or more of the following groups of amino acid residues: (a) Ile 295, Ile 296, Leu 315, Trp 316, Leu 319, Phe 355, and Leu 356; (b) Val 687, Ile 696, Leu 726, Phe 743, Trp 365, and

Ile 364; (c) Asn 684, Arg 700, and Glu 323; (d) Arg 485, Arg 467, Arg 534, Tyr 548; (e) Trp 426, Arg 485, Thr 441, and Thr 465; (f) Trp 426, Trp 717, Thr 386, and Val 384; (g) Tyr 574, Thr 386 and Val 384; (h) Tyr 574, Met 590, and Leo 634; and (i) the corresponding residues in Cdc4 homologs, paralogs, variants, or precursors. Preferably the atoms of the amino acid residues have the structural coordinates as set out in Table 6.

5 A crystal of the invention may enable the determination of structural data for a substrate or ligand. In order to be able to derive structural data for a ligand, or substrate it is necessary for the molecule to have sufficiently strong electron density to enable a model of the molecule to be built using standard techniques. For example, there should be sufficient electron density to allow a model to be built using XTALVIEW (McRee 1992 J. Mol. Graphics. 10 44-46).

10 A crystal of the invention may belong to space group $P3_2$. The term "space group" refers to the lattice and symmetry of the crystal. In a space group designation the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the contents of the asymmetric unit without changing its appearance.

15 A crystal of the invention may comprise a unit cell having the following unit dimensions: $a = 107.7 \text{ \AA}$, $b = 107.7 \text{ \AA}$, $c = 168.3 \text{ \AA}$, $\alpha = \gamma = 90^\circ$, $\beta = 120^\circ$. The term "unit cell" refers to the smallest and simplest volume element (i.e. parallelepiped-shaped block) of a crystal that is completely representative of the unit of pattern of the crystal. The unit cell axial lengths are represented by a, b, and c. Those of skill in the art understand that a set of atomic coordinates determined by X-ray crystallography is not without standard error.

20 In a preferred embodiment, a crystal of the invention has the structural coordinates as shown in Table 6. As used herein, the term "structural coordinates" refers to a set of values that define the position of one or more amino acid residues with reference to a system of axes. The term refers to a data set that defines the three dimensional structure of a molecule or molecules (e.g. Cartesian coordinates, temperature factors, and occupancies). Structural coordinates can be slightly modified and still render nearly identical three dimensional structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural coordinates that render three dimensional structures (in particular a three dimensional structure of a ligand binding pocket) that deviate from one another by a root-mean-square deviation of less than 5 Å, 4 Å, 3 Å, 2 Å, 1.5 Å, 1.0 Å, or 0.5 Å may be viewed by a person of ordinary skill in the art as very similar.

30 Variations in structural coordinates may be generated because of mathematical manipulations of the structural coordinates of a structure or binding pocket described herein. For example, the structural coordinates of Table 6 may be manipulated by crystallographic permutations of the structural coordinates, fractionalization of the structural coordinates, integer additions or subtractions to sets of the structural coordinates, inversion of the structural coordinates or any combination of the above.

35 Variations in the crystal structure due to mutations, additions, substitutions, and/or deletions of the amino acids, or other changes in any of the components that make up the crystal may also account for modifications in structural coordinates. If such modifications are within an acceptable standard error as compared to the original structural coordinates, the resulting structure may be the same. Therefore, a ligand that bound to a binding pocket of

an F-box protein, would also be expected to bind to another binding pocket whose structural coordinates defined a shape that fell within the acceptable error. Such modified structures of a binding pocket thereof are also within the scope of the invention.

Various computational analyses may be used to determine whether a molecule or the binding pocket thereof is sufficiently similar to all or parts of an F-box or a binding pocket thereof. Such analyses may be carried out using conventional software applications and methods as described herein.

A crystal of the invention may also be specifically characterised by the parameters, diffraction statistics and/or refinement statistics set out in Table 1 or in Table 2.

Illustrations of particular crystals of the invention are shown in Figures 2, 3, 4, 6 and 7.

METHOD OF MAKING A CRYSTAL

The present invention also provides a method of making a crystal according to the invention. The crystal may be formed from an aqueous solution comprising a purified polypeptide comprising an F-box protein including a variant, part, homolog, or fragment thereof (e.g. a binding pocket). A method may utilize a purified polypeptide comprising a binding pocket to form a crystal. A method may utilize one or more purified mutant polypeptides as described herein. In an embodiment, a mutant *cdc4* polypeptide is used to make crystals.

The term "purified" in reference to a polypeptide, does not require absolute purity such as a homogenous preparation rather it represents an indication that the polypeptide is relatively purer than in the natural environment. Generally, a purified polypeptide is substantially free of other proteins, lipids, carbohydrates, or other materials with which it is naturally associated, preferably at a functionally significant level for example at least 85% pure, more preferably at least 95% pure, most preferably at least 99% pure. A skilled artisan can purify a polypeptide comprising using standard techniques for protein purification. A substantially pure polypeptide will yield a single major band on a non-reducing polyacrylamide gel. Purity of the polypeptide can also be determined by amino-terminal amino acid sequence analysis.

A polypeptide used in the method may be chemically synthesized in whole or in part using techniques that are well-known in the art. Alternatively, methods are well known to the skilled artisan to construct expression vectors containing a native or mutated protein coding sequence and appropriate transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques, and *in vivo* recombination/genetic recombination. See for example the techniques described in Sambrook et al. (Molecular Cloning: A Laboratory Manual, 2nd Edition, Cold Spring Harbor Laboratory press (1989)), and other laboratory textbooks. (See also Sarker et al, Glycoconjugate J. 7:380, 1990; Sarker et al, Proc. Natl. Acad. Sci. USA 88:234-238, 1991, Sarker et al, Glycoconjugate J. 11: 204-209, 1994; Hull et al, Biochem Biophys Res Commun 176:608, 1991 and Pownall et al, Genomics 12:699-704, 1992).

Crystals may be grown from an aqueous solution containing the purified polypeptide by a variety of conventional processes. These processes include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. (See for example, McPherson, 1982 John Wiley, New York; McPherson, 1990, Eur. J. Biochem. 189: 1-23;

Webber. 1991, Adv. Protein Chem. 41:1-36). Generally, native crystals of the invention are grown by adding precipitants to the concentrated solution of the polypeptide. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

Derivative crystals of the invention can be obtained by soaking native crystals in a solution containing salts of heavy metal atoms. A complex of the invention can be obtained by soaking a native crystal in a solution containing a compound that binds the polypeptide, or they can be obtained by co-crystallizing the polypeptide in the presence of one or more compounds. In order to obtain co-crystals with a compound which binds deep within the tertiary structure of the polypeptide it is necessary to use the second method.

Once the crystal is grown it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection device. Collection of X-ray diffraction patterns are well documented by those skilled in the art (See for example, Ducruix and Geige, 1992, IRL Press, Oxford, England). A beam of X-rays enter the crystal and diffract from the crystal. An X-ray detection device can be utilized to record the diffraction patterns emanating from the crystal. Suitable devices include the Marr 345 imaging plate detector system with an RU200 rotating anode generator.

Multiwavelength anomalous diffraction (MAD) phasing using selenomethionyl (SeMet) proteins may be used to determine a crystal of the invention. Thus, the invention contemplates a method for determining a crystal structure of the invention using a selenomethionyl derivative of an F-box protein or SCF complex, including a variant, part, homolog or fragment thereof.

Methods for obtaining the three dimensional structure of the crystalline form of a molecule or complex are described herein and known to those skilled in the art (see Ducruix and Geige 1992, IRL Press, Oxford, England). Generally, the x-ray crystal structure is given by the diffraction patterns. Each diffraction pattern reflection is characterized as a vector and the data collected at this stage determines the amplitude of each vector. The phases of the vectors may be determined by the isomorphous replacement method where heavy atoms soaked into the crystal are used as reference points in the X-ray analysis (see for example, Otwinowski, 1991, Daresbury, United Kingdom, 80-86). The phases of the vectors may also be determined by molecular replacement (see for example, Naraza, 1994, Proteins 11:281-296). The amplitudes and phases of vectors from the crystalline form determined in accordance with these methods can be used to analyze other related crystalline polypeptides.

The unit cell dimensions and symmetry, and vector amplitude and phase information can be used in a Fourier transform function to calculate the electron density in the unit cell i.e. to generate an experimental electron density map. This may be accomplished using the PHASES package (Furey, 1990). Amino acid sequence structures are fit to the experimental electron density map (i.e. model building) using computer programs (e.g. Jones, TA. et al, Acta Crystallogr A47, 100-119, 1991). This structure can also be used to calculate a theoretical electron density map. The theoretical and experimental electron density maps can be compared and the agreement between the maps can be described by a parameter referred to as R-factor. A high degree of overlap in the maps is represented by a low value

R-factor. The R-factor can be minimized by using computer programs that refine the structure to achieve agreement between the theoretical and observed electron density map. For example, the XPLOR program, developed by Brunger (1992, Nature 355:472-475) can be used for model refinement.

A three dimensional structure of the molecule or complex may be described by atoms that fit the theoretical electron density characterized by a minimum R value. Files can be created for the structure that defines each atom by coordinates in three dimensions.

MUTANT CDC4 POLYPEPTIDES

The present invention provides novel mutant cdc4 polypeptides.

A particular mutant of the present invention is a polypeptide having an amino acid sequence of a cdc4 polypeptide wherein amino acid residues are replaced or deleted providing a cdc4 polypeptide that can be produced by recombinant techniques and retains its activity, for example its ability to associate with a CPD motif.

In an aspect a cdc4 sequence is mutated by deleting the region from the beginning of the F-box domain to the end of the WD40 repeat domain. In particular, terminal residues 1 to 262 and 745 to 779 can be deleted from the cdc4 sequence.

Other additions, substitutions, and/or deletions may be made to the cdc4 mutants of the present invention. In an embodiment cdc4 can be engineered to remove flexible loops comprising residues 601 to 604 and 609 to 624.

Particular mutant cdc4 polypeptides of the invention are also identified in Table 5.

The present invention also relates to nucleic acid molecules or polynucleotides encoding a cdc4 mutant polypeptide. The polynucleotides can be used to transform host cells to express the cdc4 mutant polypeptides of the invention. They can also be used as a probe to detect related enzymes.

The present invention still further relates to recombinant vectors that include the nucleic acid molecules of the invention. The nucleic acid molecules of the invention may be inserted into an appropriate vector, and the vector may contain the necessary elements for the transcription and translation of an inserted coding sequence. Accordingly, vectors may be constructed which comprise a nucleic acid molecule of the invention, and where appropriate one or more transcription and translation elements linked to the nucleic acid molecule. A vector can be used to transform host cells. Therefore, the invention provides host cells containing a vector of the invention. As well, the invention provides methods of making such vectors and host cells.

The mutant cdc4 polypeptides of the invention can be encoded, expressed, and purified by any one of a number of methods known to those skilled in the art. Preferred production methods will depend on many factors including the costs and availability of materials and other economic considerations. The optimum production procedure for a given situation will be apparent to those skilled in the art through minimal experimentation.

In accordance with an aspect of the present invention, there is provided a process for producing a cdc4 mutant polypeptide by recombinant techniques utilizing the nucleic acid molecules of the invention. The method may comprise culturing recombinant host cells containing a nucleic acid sequence encoding a cdc4 mutant polypeptide,

under conditions promoting expression of the cdc4 mutant polypeptide, and subsequent recovery of the cdc4 mutant polypeptide.

The invention further broadly contemplates a recombinant cdc4 mutant polypeptide obtained using a method of the invention.

5 A cdc4 mutant polypeptide of the invention may be conjugated with other molecules, such as polypeptides, to prepare fusion polypeptides or chimeric polypeptides. This may be accomplished, for example, by the synthesis of N-terminal or C-terminal fusion polypeptides.

10 The invention further contemplates antibodies having specificity against a cdc4 mutant polypeptide of the invention. Antibodies may be labeled with a detectable substance and used to detect cdc4 mutant polypeptides. In another embodiment, the invention provides an isolated antibody that binds specifically to a cdc4 mutant polypeptide.

 The cdc4 mutant polypeptides of the present invention are particularly well suited for use in screening methods for identifying modulators of cdc4 or SCF complexes.

15 Still further the invention provides a method for evaluating a test compound for its ability to modulate the biological activity of a cdc4 polypeptide. In this application, "modulate" refers to a change or an alteration in the biological activity of a cdc4 polypeptide. Modulation may be an increase or a decrease in activity, a change in characteristics (e.g. kinetic characteristics), or any other change in the biological, functional, or immunological properties of the polypeptide.

20 The substances and compounds identified using the methods of the invention, may be used to modulate the biological activity of a cdc4 polypeptide or a SCF complex, and they may be used in the treatment of conditions mediated by a cdc4 polypeptide or SCF complex. Accordingly, the substances and compounds may be formulated into compositions for administration to individuals suffering from one or more of these conditions. Therefore, the present invention also relates to a composition comprising one or more of a substance or compound identified using a method of the invention, and a pharmaceutically acceptable carrier, excipient or diluent. A method for treating or preventing these conditions is also provided comprising administering to a patient in need thereof, a composition of the invention.

25 **MODEL**

30 A crystal structure of the present invention may be used to make a model of a binding pocket of a SCF E3 ubiquitin ligase, in particular an F-box protein, that is involved in substrate selection and/or orientation. A model may, for example, be a structural model or a computer model. A model may represent the secondary, tertiary and/or quaternary structure of the binding pocket. The model itself may be in two or three dimensions. It is possible for a computer model to be in three dimensions despite the constraints imposed by a conventional computer screen, if it is possible to scroll along at least a pair of axes, causing "rotation" of the image.

35 As used herein, the term "modelling" includes the quantitative and qualitative analysis of molecular structure and/or function based on atomic structural information and interaction models. The term "modelling" includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models.

Preferably, modelling is performed using a computer and may be further optimized using known methods. This is called modelling optimisation.

An integral step to an approach of the invention for designing modulators (e.g. inhibitors) of a subject F-box protein or SCF complex involves construction of computer graphics models of a binding pocket of the invention which can be used to design pharmacophores by rational drug design. For instance, for an inhibitor to interact optimally with the subject binding pocket, it will generally be desirable that it have a shape which is at least partly complimentary to that of a particular binding pocket of the protein, as for example those binding pockets of the protein which are involved in recognition of a ligand (e.g. substrate). Additionally, other factors, including electrostatic interactions, hydrogen bonding, hydrophobic interactions, desolvation effects, and cooperative motions of ligand and receptor, all influence the binding effect and should be taken into account in attempts to design bioactive modulators (e.g. inhibitors).

As described herein, a computer-generated molecular model of the subject binding pockets can be created. In preferred embodiments, at least the C α -carbon positions of the binding pockets are mapped to a particular coordinate pattern, such as the coordinates for a binding pocket in Table 6, by homology modeling, and the structure of the protein and velocities of each atom are calculated at a simulation temperature (T_0) at which the docking simulation is to be determined. Typically, such a protocol involves primarily the prediction of side-chain conformations in the modeled binding pocket, while assuming a main-chain trace taken from a tertiary structure such as provided in Table 6 and the Figures. Computer programs for performing energy minimization routines are commonly used to generate molecular models. For example, both the CHARMM (Brooks et al. (1983) *J Comput Chem* 4:187-217) and AMBER (Weiner et al (1981) *J. Comput. Chem.* 106: 765) algorithms handle all of the molecular system setup, force field calculation, and analysis (see also, Eisenfield et al. (1991) *Am J Physiol* 261:C376-386; Lybrand (1991) *J Pharm Belg* 46:49-54; Froimowitz (1990) *Biotechniques* 8:640-644; Burbam et al. (1990) *Proteins* 7:99-111; Pedersen (1985) *Environ Health Perspect* 61:185-190; and Kini et al. (1991) *J Biomol Struct Dyn* 9:475-488). At the heart of these programs is a set of subroutines that, given the position of every atom in the model, calculate the total potential energy of the system and the force on each atom. These programs may utilize a starting set of atomic coordinates, such as the coordinates provided in Table 6, the parameters for the various terms of the potential energy function, and a description of the molecular topology (the covalent structure). Common features of such molecular modeling methods include: provisions for handling hydrogen bonds and other constraint forces; the use of periodic boundary conditions; and provisions for occasionally adjusting positions, velocities, or other parameters in order to maintain or change temperature, pressure, volume, forces of constraint, or other externally controlled conditions.

Most conventional energy minimization methods use the input data described above and the fact that the potential energy function is an explicit, differentiable function of Cartesian coordinates, to calculate the potential energy and its gradient (which gives the force on each atom) for any set of atomic positions. This information can be used to generate a new set of coordinates in an effort to reduce the total potential energy and, by repeating this process

over and over, to optimize the molecular structure under a given set of external conditions. These energy minimization methods are routinely applied to molecules similar to the subject proteins as well as nucleic acids, polymers and zeolites.

In general, energy minimization methods can be carried out for a given temperature, T_i , which may be different than the docking simulation temperature, T_o . Upon energy minimization of the molecule at T_i , coordinates and velocities of all the atoms in the system are computed. Additionally, the normal modes of the system are calculated. It will be appreciated by those skilled in the art that each normal mode is a collective, periodic motion, with all parts of the system moving in phase with each other, and that the motion of the molecule is the superposition of all normal modes. For a given temperature, the mean square amplitude of motion in a particular mode is inversely proportional to the effective force constant for that mode, so that the motion of the molecule will often be dominated by the low frequency vibrations.

After the molecular model has been energy minimized at T_i , the system is "heated" or "cooled" to the simulation temperature, T_o , by carrying out an equilibration run where the velocities of the atoms are scaled in a step-wise manner until the desired temperature, T_o , is reached. The system is further equilibrated for a specified period of time until certain properties of the system, such as average kinetic energy, remain constant. The coordinates and velocities of each atom are then obtained from the equilibrated system.

Further energy minimization routines can also be carried out. For example, a second class of methods involves calculating approximate solutions to the constrained EOM for the protein. These methods use an iterative approach to solve for the Lagrange multipliers and, typically, only need a few iterations if the corrections required are small. The most popular method of this type, SHAKE (Ryckaert et al. (1977) *J Comput Phys* 23:327; and Van Gunsteren et al. (1977) *Mol Phys* 34:1311) is easy to implement and scales as $O(N)$ as the number of constraints increases. Therefore, the method is applicable to macromolecules such as F-box proteins. An alternative method, RATTLE (Anderson (1983) *J Comput Phys* 52:24) is based on the velocity version of the Verlet algorithm. Like SHAKE, RATTLE is an iterative algorithm and can be used to energy minimize the model of the subject protein.

Overlays and super positioning with a three dimensional model of a binding pocket of the invention may be used for modelling optimisation. Additionally alignment and/or modelling can be used as a guide for the placement of mutations on a binding pocket to characterize the nature of the site in the context of a cell.

The three dimensional structure of a new crystal may be modelled using molecular replacement. The term "molecular replacement" refers to a method that involves generating a preliminary model of a molecule or complex whose structural coordinates are unknown, by orienting and positioning a molecule whose structural coordinates are known within the unit cell of the unknown crystal, so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. Lattman, E., "Use of

the Rotation and Translation Functions", in *Methods in Enzymology*, 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", *Int. Sci. Rev. Ser.*, No. 13, Gordon & Breach, New York, (1972).

Commonly used computer software packages for molecular replacement are X-PLOR (Brunger 1992, *Nature* 355: 472-475), AMoRE (Navaza, 1994, *Acta Crystallogr.* A50:157-163), the CCP4 package (Collaborative Computational Project, Number 4, "The CCP4 Suite: Programs for Protein Crystallography", *Acta Cryst.*, Vol. D50, pp. 760-763, 1994), the MERLOT package (P.M.D. Fitzgerald, *J. Appl. Cryst.*, Vol. 21, pp. 273-278, 1988) and XTALVIEW (McCree et al (1992) *J. Mol. Graphics* 10: 44-46. It is preferable that the resulting structure not exhibit a root-mean-square deviation of more than 3 Å.

Molecular replacement computer programs generally involve the following steps: (1) determining the number of molecules in the unit cell and defining the angles between them (self rotation function); (2) rotating the known structure against diffraction data to define the orientation of the molecules in the unit cell (rotation function); (3) translating the known structure in three dimensions to correctly position the molecules in the unit cell (translation function); (4) determining the phases of the X-ray diffraction data and calculating an R-factor calculated from the reference data set and from the new data wherein an R-factor between 30-50% indicates that the orientations of the atoms in the unit cell have been reasonably determined by the method; and (5) optionally, decreasing the R-factor to about 20% by refining the new electron density map using iterative refinement techniques known to those skilled in the art (refinement).

The quality of the model may be analysed using a program such as PROCHECK or 3D-Profiler [Laskowski et al 1993 *J. Appl. Cryst.* 26:283-291; Luthy R. et al, *Nature* 356: 83-85, 1992; and Bowie, J.U. et al, *Science* 253: 164-170, 1991]. Once any irregularities have been resolved, the entire structure may be further refined.

Other molecular modelling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. *et al*, "Molecular Modelling Software and Methods for Medicinal Chemistry", *J. Med. Chem.*, 33, pp. 883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", *Current Opinions in Structural Biology*, 2, pp. 202-210 (1992).

Using the structural coordinates of crystal provided by the invention, molecular modelling may be used to determine the structural coordinates of a crystalline mutant or homolog of a SCF complex or F-box binding pocket involved in substrate selection and/or orientation. By the same token a crystal of the invention can be used to provide a model of a substrate or ligand. Modelling techniques can then be used to approximate the three dimensional structure of substrate or ligand derivatives and other components which may be able to mimic the atomic contacts between a substrate or ligand and binding pocket.

COMPUTER FORMAT OF CRYSTALS/MODELS

Information derivable from a crystal of the present invention (for example the structural coordinates) and/or the model of the present invention may be provided in a computer-readable format.

Therefore, the invention provides a computer readable medium or a machine readable storage medium which comprises the structural coordinates of a binding pocket of an SCF complex of F box protein described herein

including all or any parts thereof, or substrates or ligands including portions thereof. Such storage medium or storage medium encoded with these data are capable of displaying on a computer screen or similar viewing device, a three-dimensional graphical representation of a molecule or molecular complex which comprises such binding pockets or similarly shaped homologous binding pockets. Thus, the invention also provides computerized representations of the secondary or three-dimensional structures of a binding pocket of the invention, including any electronic, magnetic, or electromagnetic storage forms of the data needed to define the structures such that the data will be computer readable for purposes of display and/or manipulation.

In an aspect the invention provides a computer for producing a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a binding pocket defined by structural coordinates of a binding pocket or structural coordinates of atoms of a substrate or ligand, or a three-dimensional representation of a homolog of said molecule or molecular complex, wherein said homolog comprises a binding pocket, or substrate or ligand that has a root mean square deviation from the backbone atoms not more than 1.5 angstroms wherein said computer comprises:

- (a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates of a binding pocket or a substrate according to Table 6;
- (b) a working memory for storing instructions for processing said machine-readable data;
- (c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and
- (d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

The invention also provides a computer for determining at least a portion of the structural coordinates corresponding to an X-ray diffraction pattern of a molecule or molecular complex wherein said computer comprises:

- (a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates according to Table 6;
- (b) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises an X-ray diffraction pattern of said molecule or molecular complex;
- (c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);
- (d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structural coordinates; and
- (e) a display coupled to said central-processing unit for displaying said structural coordinates of said molecule or molecular complex.

STRUCTURAL STUDIES

The present invention also provides a method for determining the secondary and/or tertiary structures of a polypeptide or part or complexes thereof by using a crystal, or a model according to the present invention. The polypeptide or part thereof may be any polypeptide or part thereof for which the secondary and or tertiary structure is uncharacterised or incompletely characterised. In a preferred embodiment the polypeptide shares (or is predicted to share) some structural or functional homology to a crystal of the present invention. For example, the polypeptide may show a degree of structural homology over some or all parts of the primary amino acid sequence.

The polypeptide may be an F-box protein, or part thereof with a different specificity for a substrate. Alternatively (or in addition) the polypeptide may be an F-box protein from a different species.

The polypeptide may be a mutant of a wild-type F-box protein. A mutant may arise naturally, or may be made artificially (for example using molecular biology techniques). The mutant may also not be “made” at all in the conventional sense, but merely tested theoretically using the model of the present invention. A mutant may or may not be functional.

Thus, using a model of the present invention, the effect of a particular mutation on the overall two and/or three dimensional structure of an F-box protein or SCF complex or the interaction between a binding pocket of an F-box protein or SCF complex and a substrate or ligand can be investigated.

Alternatively, the polypeptide may perform an analogous function or be suspected to show a similar mechanism to an F-box protein.

The polypeptide may also be the same as the polypeptide of the crystal, but in association with a different substrate or ligand (for example, modulator or inhibitor) or cofactor. In this way it is possible to investigate the effect of altering the substrate or ligand with which the polypeptide is associated on the structure of the binding pocket.

Secondary or tertiary structure may be determined by applying the structural coordinates of a crystal or model of the present invention to other data such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Homology modeling, molecular replacement, and nuclear magnetic resonance methods using these other data sets are described below.

Homology modeling (also known as comparative modeling or knowledge-based modeling) methods develop a three dimensional model from a polypeptide sequence based on the structures of known proteins (i.e. an F-box structure or complex thereof described herein). The method utilizes a computer model of a crystal of the present invention (the “known structure”), a computer representation of the amino acid sequence of the polypeptide with an unknown structure, and standard computer representations of the structures of amino acids. The method in particular comprises the steps of; (a) identifying structurally conserved and variable regions in the known structure; (b) aligning the amino acid sequences of the known structure and unknown structure (c) generating co-ordinates of main chain atoms and side chain atoms in structurally conserved and variable regions of the unknown structure based on the coordinates of the known structure thereby obtaining a homology model; and (d) refining the homology model to obtain a three dimensional structure for the unknown structure. This method is well known to those skilled in the art

(Greer, 1985, Science 228, 1055; Bundell et al 1988, Eur. J. Biochem. 172, 513; Knighton et al., 1992, Science 258:130-135, <http://biochem.vt.edu/courses/modeling/homology.htm>). Computer programs that can be used in homology modelling are Quanta and the Homology module in the Insight II modelling package distributed by Molecular Simulations Inc, or MODELLER (Rockefeller University, www.iucr.ac.uk/sinris-top/logical/prg-modeller.html).

In step (a) of the homology modelling method, a known structure is examined to identify the structurally conserved regions (SCRs) from which an average structure, or framework, can be constructed for these regions of the protein. Variable regions (VRs), in which known structures may differ in conformation, also must be identified. SCRs generally correspond to the elements of secondary structure, such as alpha-helices and beta-sheets, and to ligand- and substrate-binding sites. The VRs usually lie on the surface of the proteins and form the loops where the main chain turns.

Many methods are available for sequence alignment of known structures and unknown structures. Sequence alignments generally are based on the dynamic programming algorithm of Needleman and Wunsch [J. Mol. Biol. 48: 442-453, 1970]. Current methods include FASTA, Smith-Waterman, and BLASTP, with the BLASTP method differing from the other two in not allowing gaps. Scoring of alignments typically involves construction of a 20x20 matrix in which identical amino acids and those of similar character (i.e., conservative substitutions) may be scored higher than those of different character. Substitution schemes which may be used to score alignments include the scoring matrices PAM (Dayhoff et al., Meth. Enzymol. 91: 524-545, 1983), and BLOSUM (Henikoff and Henikoff, Proc. Nat. Acad. Sci. USA 89: 10915-10919, 1992), and the matrices based on alignments derived from three-dimensional structures including that of Johnson and Overington (JO matrices) (J. Mol. Biol. 233: 716-738, 1993).

Alignment based solely on sequence may be used; however, other structural features also may be taken into account. In Quanta, multiple sequence alignment algorithms are available that may be used when aligning a sequence of the unknown with the known structures. Four scoring systems (i.e. sequence homology, secondary structure homology, residue accessibility homology, CA-CA distance homology) are available, each of which may be evaluated during an alignment so that relative statistical weights may be assigned.

When generating coordinates for the unknown structure, main chain atoms and side chain atoms, both in SCRs and VRs need to be modelled. A variety of approaches known to those skilled in the art may be used to assign co-ordinates to the unknown. In particular, the co-ordinates of the main chain atoms of SCRs will be transferred to the unknown structure. VRs correspond most often to the loops on the surface of the polypeptide and if a loop in the known structure is a good model for the unknown, then the main chain co-ordinates of the known structure may be copied. Side chain coordinates of SCRs and VRs are copied if the residue type in the unknown is identical to or very similar to that in the known structure. For other side chain coordinates, a side chain rotamer library may be used to define the side chain coordinates. When a good model for a loop cannot be found fragment databases may be searched for loops in other proteins that may provide a suitable model for the unknown. If desired, the loop may then be subjected to conformational searching to identify low energy conformers if desired.

Once a homology model has been generated it is analyzed to determine its correctness. A computer program available to assist in this analysis is the Protein Health module in Quanta which provides a variety of tests. Other programs that provide structure analysis along with output include PROCHECK and 3D-Profiler [Luthy R. et al, Nature 356: 83-85, 1992; and Bowie, J.U. et al, Science 253: 164-170, 1991]. Once any irregularities have been resolved, the entire structure may be further refined. Refinement may consist of energy minimization with restraints, especially for the SCRs. Restraints may be gradually removed for subsequent minimizations. Molecular dynamics may also be applied in conjunction with energy minimization.

Molecular replacement involves applying a known structure to solve the X-ray crystallographic data set of a polypeptide of unknown structure. The method can be used to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. Thus in an embodiment of the invention, a method is provided for determining three dimensional structures of polypeptides with unknown structure by applying the structural coordinates of a crystal of the present invention to provide an X-ray crystallographic data set for a polypeptide of unknown structure, and (b) determining a low energy conformation of the resulting structure.

The structural coordinates of a crystal of the present invention may be applied to nuclear magnetic resonance (NMR) data to determine the three dimensional structures of polypeptides with uncharacterised or incompletely characterised structure. (See for example, Wuthrich, 1986, John Wiley and Sons, New York: 176-199; Pflugrath et al., 1986, J. Molecular Biology 189: 383-386; Kline et al., 1986 J. Molecular Biology 189:377-382). While the secondary structure of a polypeptide may often be determined by NMR data, the spatial connections between individual pieces of secondary structure are not as readily determined. The structural coordinates of a polypeptide defined by X-ray crystallography can guide the NMR spectroscopist to an understanding of the spatial interactions between secondary structural elements in a polypeptide of related structure. Information on spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from two-dimensional NMR experiments. In addition, applying the structural coordinates after the determination of secondary structure by NMR techniques simplifies the assignment of NOE's relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure.

In an embodiment, the invention relates to a method of determining three dimensional structures of polypeptides with unknown structures, by applying the structural coordinates of a crystal of the present invention to nuclear magnetic resonance (NMR) data of the unknown structure. This method comprises the steps of: (a) determining the secondary structure of an unknown structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The term "through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence. The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

SCREENING METHODS

Another aspect of the present invention is the design and identification of agents that inhibit or potentiate an interaction between an F-box protein or an SCF E3 ubiquitin ligase and a substrate. The rationale design and identification of agents can be accomplished by utilizing the structural coordinates that define a binding pocket of the present invention involved in substrate selection and/or orientation.

The structures described herein, and the structures of other polypeptides determined by homology modeling, molecular replacement, and NMR techniques described herein can also be applied to modulator design and identification methods.

The invention contemplates molecular models, in particular three-dimensional molecular models of binding pockets of the present invention involved in substrate selection and/or orientation, and their use as templates for the design of agents able to mimic or inhibit substrate binding (e.g. modulators).

In certain embodiments, the present invention provides a method of screening for a ligand that associates with a binding pocket and/or modulates the function of a F-box protein or SCF complex by using a crystal or a model according to the present invention. The method may involve investigating whether a test compound is capable of associating with or binding a binding pocket, and/or inhibiting or enhancing interactions of atomic contacts in a binding pocket.

In accordance with an aspect of the present invention, a method is provided for screening for a ligand capable of binding to a binding pocket, wherein the method comprises using a crystal or model according to the invention.

In another aspect, the invention relates to a method of screening for a ligand capable of binding to a binding pocket, wherein the binding pocket is defined by the structural coordinates given herein, the method comprising contacting the binding pocket with a test compound and determining if the test compound binds to the binding pocket.

In one embodiment, the present invention provides a method of screening for a test compound capable of interacting with one or more key amino acid residues of a binding pocket of the present invention. For example, a test compound that interacts with one or more of amino acids of a binding pocket may prevent interaction of the F-box protein or complex thereof and its substrate resulting in modification of the SCF E3 ubiquitin ligase activity.

Another aspect of the invention provides a process comprising the steps of:

- (a) performing a method of screening for a ligand described above;
- (b) identifying one or more ligands capable of binding to a binding pocket; and
- (c) preparing a quantity of said one or more ligands.

A further aspect of the invention provides a process comprising the steps of;

- (a) performing a method of screening for a ligand as described above;
- (b) identifying one or more ligands capable of binding to a binding pocket; and
- (c) preparing a pharmaceutical composition comprising said one or more ligands.

Once a test compound capable of interacting with one or more key amino acid residues in a binding pocket of the present invention has been identified, further steps may be carried out either to select and/or modify compounds

and/or to modify existing compounds, to modulate the interaction with the key amino acid residues in the binding pocket.

Yet another aspect of the invention provides a process comprising the steps of;

- (a) performing the method of screening for a ligand as described above;
- (b) identifying one or more ligands capable of binding to a binding pocket;
- (c) modifying said one or more ligands capable of binding to a binding pocket;
- (d) performing said method of screening for a ligand as described above; and
- (e) optionally preparing a pharmaceutical composition comprising said one or more ligands.

In another aspect of the invention, a method of screening for a test compound is provided comprising screening for test compounds that affect (inhibit or potentiate) an interaction between an F-box protein or SCF complex and a substrate as defined by interactions 1 to 4 or 5 to 8/9 in Table 3 or Table 4.

As used herein, the term "test compound" means any compound which is potentially capable of associating with a binding pocket, inhibiting or enhancing interactions of atomic contacts in a binding pocket. If, after testing, it is determined that the test compound does bind to the binding pocket, inhibits or enhances interactions of atomic contacts in a binding pocket, it is known as a "ligand".

The test compound may be designed or obtained from a library of compounds which may comprise peptides, as well as other compounds, such as small organic molecules and particularly new lead compounds. By way of example, the test compound may be a natural substance, a biological macromolecule, or an extract made from biological materials such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic test compound, a semi-synthetic test compound, a carbohydrate, a monosaccharide, an oligosaccharide or polysaccharide, a glycolipid, a glycopeptide, a saponin, a heterocyclic compound, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised test compound, a peptide cleaved from a whole protein, or a peptide synthesised synthetically (such as, by way of example, either using a peptide synthesizer or by recombinant techniques or combinations thereof), a recombinant test compound, a natural or a non-natural test compound, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof.

The increasing availability of biomacromolecule structures of potential pharmacophoric molecules that have been solved crystallographically has prompted the development of a variety of direct computational methods for molecular design, in which the steric and electronic properties of substrate binding sites are used to guide the design of potential ligands (Cohen et al. (1990) *J. Med. Cam.* 33: 883-894; Kuntz et al. (1982) *J. Mol. Biol* 161: 269-288; DesJarlais (1988) *J. Med. Cam.* 31: 722-729; Bartlett et al. (1989) (*Spec. Publ., Roy. Soc. Chem.*) 78: 182-196; Goodford et al. (1985) *J. Med. Cam.* 28: 849-857; DesJarlais et al. *J. Med. Cam.* 29: 2149-2153). Directed methods generally fall into two categories: (1) design by analogy in which 3-D structures of known molecules (such as from a crystallographic database) are docked to the structure and scored for goodness-of-fit; and (2) *de novo* design, in which the ligand model is constructed piece-wise. The latter approach, in particular, can facilitate the development of novel molecules, uniquely designed to bind to the subject binding pockets.

The test compound may be screened as part of a library or a data base of molecules. Modulators of a binding pocket of the present invention may be identified by docking a computer representation of compounds from one or more database of molecules. Data bases which may be used include ACD (Molecular Designs Limited), NCI (National Cancer Institute), CCDC (Cambridge Crystallographic Data Center), CAST (Chemical Abstract Service), Derwent (Derwent Information Limited), Maybridge (Maybridge Chemical Company Ltd), Aldrich (Aldrich Chemical Company), DOCK (University of California in San Francisco), and the Directory of Natural Products (Chapman & Hall). Computer programs such as CONCORD (Tripos Associates) or DB-Converter (Molecular Simulations Limited) can be used to convert a data set represented in two dimensions to one represented in three dimensions.

Test compounds may tested for their capacity to fit spatially into a binding pocket. As used herein, the term “fits spatially” means that the three-dimensional structure of the test compound is accommodated geometrically in a cavity of a binding pocket. The test compound can then be considered to be a ligand.

A favourable geometric fit occurs when the surface area of the test compound is in close proximity with the surface area of the cavity of a binding pocket without forming unfavorable interactions. A favourable complementary interaction occurs where the test compound interacts by hydrophobic, aromatic, ionic, dipolar, or hydrogen donating and accepting forces. Unfavourable interactions may be steric hindrance between atoms in the test compound and atoms in the binding pocket.

If a model of the present invention is a computer model, the test compounds may be positioned in a binding pocket through computational docking. If, on the other hand, the model of the present invention is a structural model, the test compounds may be positioned in the binding pocket by, for example, manual docking.

As used herein the term “docking” refers to a process of placing a compound in close proximity with a binding pocket, or a process of finding low energy conformations of a test compound/ binding pocket complex.

A screening method of the present invention may comprise the following steps:

- (i) generating a computer model of a binding pocket using a crystal according to the invention;
- (ii) docking a computer representation of a test compound with the computer model; and
- (iii) analysing the fit of the compound in the binding pocket.

In an aspect of the invention, a method is provided comprising the following steps:

- (a) docking a computer representation of a structure of a test compound into a computer representation of a binding pocket defined in accordance with the invention using a computer program, or by interactively moving the representation of the test compound into the representation of the binding pocket;
- (b) characterizing the geometry and the complementary interactions formed between the atoms of the binding pocket and the compound; optionally
- (c) searching libraries for molecular fragments which can fit into the empty space between the compound and the binding pocket and can be linked to the compound; and

- (d) linking the fragments found in (c) to the compound and evaluating the new modified compound.

In an embodiment of the invention, a method is provided which comprises the following steps:

- (a) docking a computer representation of a test compound from a computer data base with a computer representation of a selected binding pocket defined in accordance with the invention to define a complex;
- (b) determining a conformation of the complex with a favorable fit and favourable complementary interactions; and
- (c) identifying test compounds that best fit the selected binding pocket as potential modulators of a F-box protein or SCF complex comprising the binding pocket.

In another embodiment of the invention, a method is provided which comprises docking a computer representation of a selected binding pocket defined by the atomic interactions, atomic contacts, or structural coordinates in accordance with the invention to define a complex. In particular a method is provided comprising:

- (a) docking a computer representation of a test compound from a computer database with a computer representation of a selected binding pocket defined by the atomic interactions, atomic contacts, or structural coordinates described herein;
- (b) determining a conformation of the complex with a favorable fit and favourable complementary interactions; and
- (c) identifying test compounds that best fit the selected binding pocket as potential modulators of the a F-box protein or SCF complex comprising the binding pocket

A model used in a screening method may comprise a binding pocket either alone or in association with one or more ligands and/or cofactors. For example, the model may comprise the binding pocket in association with a substrate (or analogue thereof), and/or modulator.

If the model comprises an unassociated binding pocket, then the selected site under investigation may be the binding pocket itself. The test compound may, for example, mimic a known ligand (e.g. substrate) for an F-box protein in order to interact with the binding pocket. The selected site may alternatively be another site on the F-box protein.

If the model comprises an associated binding pocket, for example a binding pocket in association with a substrate or ligand, the selected site may be the binding pocket or a site made up of the binding pocket and the complexed substrate or ligand, or a site on the substrate or ligand itself. The test compound may be investigated for its capacity to modulate the interaction with the associated molecule.

The screening methods described herein may be applied to a plurality of test compounds, to identify those that best fit the selected site. A test compound (or plurality of test compounds) may be selected on the basis of their similarity to a substrate or ligand for an F-box protein. For example, the screening method may comprise the following steps:

- (i) generating a computer model of a binding pocket in complex with a substrate or ligand;

- (ii) searching for a test compound with a similar three dimensional structure and/or similar chemical groups as the substrate or ligand; and
- (iii) evaluating the fit of the test compound in the binding pocket.

Searching may be carried out using a database of computer representations of potential compounds, using methods known in the art.

The present invention also provides a method for designing ligands for F-box proteins or SCF complexes. It is well known in the art to use a screening method as described above to identify a test compound with promising fit, but then to use this test compound as a starting point to design a ligand with improved fit to the model. Such techniques are known as "structure-based ligand design" (See Kuntz et al., 1994, *Acc. Chem. Res.* 27:117; Guida, 1994, *Current Opinion in Struc. Biol.* 4: 777; and Colman, 1994, *Current Opinion in Struc. Biol.* 4: 868, for reviews of structure-based drug design and identification; and Kuntz et al 1982, *J. Mol. Biol.* 162:269; Kuntz et al., 1994, *Acc. Chem. Res.* 27: 117; Meng et al., 1992, *J. Compt. Chem.* 13: 505; Bohm, 1994, *J. Comp. Aided Molec. Design* 8: 623 for methods of structure-based modulator design).

Examples of computer programs that may be used for structure-based ligand design are CAVEAT (Bartlett et al., 1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M. Ley, S.V.; Campbell, N.M. eds; Royal Society of Chemistry: Cambridge, pp 182-196); FLOG (Miller et al., 1994, *J. Comp. Aided Molec. Design* 8:153); PRO Modulator (Clark et al., 1995 *J. Comp. Aided Molec. Design* 9:13); MCSS (Miranker and Karplus, 1991, *Proteins: Structure, Fuction, and Genetics* 8:195); and, GRID (Goodford, 1985, *J. Med. Chem.* 28:849).

The method may comprise the following steps:

- (i) docking a model of a test compound with a model of a binding pocket;
- (ii) identifying one or more groups on the test compound which may be modified to improve their fit in the binding pocket;
- (iii) replacing one or more identified groups to produce a modified test compound model; and
- (iv) docking the modified test compound model with the model of the binding pocket.

Evaluation of fit may comprise the following steps:

- (a) mapping chemical features of a test compound such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites; and
- (b) adding geometric constraints to selected mapped features.

The fit of the modified test compound may then be evaluated using the same criteria.

The chemical modification of a group may either enhance or reduce hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between the test compound and the key amino acid residue(s) of the binding pocket. Preferably the group modifications involve the addition removal or replacement of substituents onto the test compound such that the substituents are positioned to collide or to bind

preferentially with one or more amino acid residues that correspond to the key amino acid residues of the binding pocket.

If a modified test compound model has an improved fit, then it may bind to a binding pocket and be considered to be a “ligand”. Rational modification of groups may be made with the aid of libraries of molecular fragments which may be screened for their capacity to fit into the available space and to interact with the appropriate atoms. Databases of computer representations of libraries of chemical groups are available commercially, for this purpose.

The test compound may also be modified “*in situ*” (i.e. once docked into the potential binding pocket), enabling immediate evaluation of the effect of replacing selected groups. The computer representation of the test compound may be modified by deleting a chemical group or groups, or by adding a chemical group or groups. After each modification to a compound, the atoms of the modified compound and potential binding pocket can be shifted in conformation and the distance between the modulator and the binding pocket atoms may be scored on the basis of geometric fit and favourable complementary interactions between the molecules. This technique is described in detail in Molecular Simulations User Manual, 1995 in LUDI.

Examples of ligand building and/or searching computer programs include programs in the Molecular Simulations Package (Catalyst), ISIS/HOST, ISIS/BASE, and ISIS/DRAW (Molecular Designs Limited), and UNITY (Tripos Associates).

The “starting point” for rational ligand design may be a known substrate or ligand. For example, in order to identify potential modulators of an F-box protein, a logical approach would be to start with a known ligand or substrate to produce a molecule which mimics the binding of the ligand or substrate. Such a molecule may, for example, act as a competitive inhibitor for the true substrate or ligand, or may bind so strongly that the interaction (and inhibition) is effectively irreversible.

Such a method may comprise the following steps:

- (i) generating a computer model of a binding pocket in complex with a substrate or ligand;
- (ii) replacing one or more groups on the ligand model to produce a modified substrate or ligand; and
- (iii) evaluating the fit of the modified substrate or ligand in the binding pocket.

The replacement groups could be selected and replaced using a compound construction program which replaces computer representations of chemical groups with groups from a computer database, where the representations of the compounds are defined by structural coordinates.

In an embodiment, a screening method is provided for identifying a substrate or ligand of an F-box protein, comprising the step of using the structural coordinates of a CPD motif defined in relation to its spatial association with a binding pocket of the invention, to generate a compound that is capable of associating with the binding pocket.

In an embodiment of the invention, a screening method is provided for identifying a ligand of an F-box protein, in particular a cdc4 protein, comprising the step of using the structural coordinates of the CPD motif listed in Table 6 to generate a compound for associating with a binding pocket of an F-box protein, in particular a cdc4 protein

as described herein. The following steps are employed in a particular method of the invention: (a) generating a computer representation of a CPD motif defined by its structural coordinates listed in Table 6; and (b) searching for molecules in a data base that are structurally or chemically similar to the defined CPD motif, using a searching computer program, or replacing portions of the CPD motif with similar chemical structures from a database using a compound building computer program.

A screening method is provided for identifying a ligand of an F-box protein, in particular a cdc4 protein, or a SCF complex comprising the step of using the structural coordinates of a binding pocket comprising a WD40 repeat or part thereof listed in Table 6 to generate a compound for associating with a F-box domain of an F-box protein. The following steps are employed in a particular method of the invention: (a) generating a computer representation of a binding pocket comprising a WD40 repeat region or part thereof defined by its structural coordinates listed in Table 6; and (b) searching for molecules in a data base that are structurally or chemically similar to the defined binding pocket using a searching computer program, or replacing portions of the binding pocket with structures from a database using a compound building computer program.

A screening method is provided for identifying a ligand of an F-box protein, in particular a cdc4 protein, of a SCF complex comprising the step of using the structural coordinates of a binding pocket comprising an F-box domain or part thereof, or helical linker listed in Table 6 to generate a compound for associating with a F-box domain or helical linker of an F-box protein. The following steps are employed in a particular method of the invention: (a) generating a computer representation of a binding pocket comprising a an F-box domain or part thereof, or helical linker defined by its structural coordinates listed in Table 4; and (b) searching for molecules in a data base that are structurally or chemically similar to the defined binding pocket using a searching computer program, or replacing portions of the binding pocket with structures from a database using a compound building computer program.

The screening methods of the present invention may be used to identify compounds or entities that associate with a molecule that associates with an F-box protein, in particular a cdc4 protein, or an SCF complex.

In an illustrative embodiment, the design of potential modulators or substrates for SCF complexes begins from the general perspective of shape complementarity for an active site and substrate specificity subsites of the receptor, and a search algorithm is employed which is capable of scanning a database of small molecules of known three-dimensional structure for candidates which fit geometrically into the target protein site. It is not expected that the molecules found in the shape search will necessarily be leads themselves, since no evaluation of chemical interaction need necessarily be made during the initial search. Rather, it is anticipated that such candidates might act as the framework for further design, providing molecular skeletons to which appropriate atomic replacements can be made. Of course, the chemical complementarity of these molecules can be evaluated, but it is expected that atom types will be changed to maximize the electrostatic, hydrogen bonding, and hydrophobic interactions with the receptor. Most algorithms of this type provide a method for finding a wide assortment of chemical structures that are complementary to the shape of a binding site of a subject molecule or complex. Each of a set of small molecules from a particular data-base, such as the Cambridge Crystallographic Data Bank (CCDB) (Allen et al. (1973) *J. Chem. Doc.*

13: 119), is individually docked to the binding pocket of the invention, in a number of geometrically permissible orientations with use of a docking algorithm. In a preferred embodiment, a set of computer algorithms called DOCK, can be used to characterize the shape of invaginations and grooves that form active sites and recognition surfaces of a subject molecule or complex(Kuntz et al. (1982) *J. Mol. Biol* 161: 269-288). The program can also search a database of small molecules for templates whose shapes are complementary to particular binding pockets or sites of a receptor (DesJarlais et al. (1988) *J Med Chem* 31: 722-729). These templates normally require modification to achieve good chemical and electrostatic interactions (DesJarlais et al. (1989) *ACS Symp Ser* 413: 60-69). However, the program has been shown to position accurately known cofactors for ligands based on shape constraints alone.

The orientations are evaluated for goodness-of-fit and the best are kept for further examination using molecular mechanics programs, such as AMBER or CHARMM. Such algorithms have previously proven successful in finding a variety of molecules that are complementary in shape to a given binding site of a molecule or complex, and have been shown to have several attractive features. First, such algorithms can retrieve a remarkable diversity of molecular architectures. Second, the best structures have, in previous applications to other proteins, demonstrated impressive shape complementarity over an extended surface area. Third, the overall approach appears to be quite robust with respect to small uncertainties in positioning of the candidate atoms.

Goodford (1985, *J Med Chem* 28:849-857) and Boobbyer et al. (1989, *J Med Chem* 32:1083-1094) have produced a computer program (GRID) which seeks to determine regions of high affinity for different chemical groups (termed probes) on the molecular surface of the binding site. GRID hence provides a tool for suggesting modifications to known ligands that might enhance binding. It may be anticipated that some of the sites discerned by GRID as regions of high affinity correspond to "pharmacophoric patterns" determined inferentially from a series of known ligands. As used herein, a pharmacophoric pattern is a geometric arrangement of features of the anticipated ligand that is believed to be important for binding. Attempts have been made to use pharmacophoric patterns as a search screen for novel ligands (Jakes et al. (1987) *J Mol Graph* 5:41-48; Brint et al. (1987) *J Mol Graph* 5:49-56; Jakes et al. (1986) *J Mol Graph* 4:12-20); however, the constraint of steric and "chemical" fit in the putative (and possibly unknown) binding pocket or site is ignored. Goodsell and Olson (1990, *Proteins: Struct Funct Genet* 8:195-202) have used the Metropolis (simulated annealing) algorithm to dock a single known ligand into a target protein. They allow torsional flexibility in the ligand and use GRID interaction energy maps as rapid lookup tables for computing approximate interaction energies. Given the large number of degrees of freedom available to the ligand, the Metropolis algorithm is time-consuming and is unsuited to searching a candidate database of a few thousand small molecules.

Yet a further embodiment of the present invention utilizes a computer algorithm such as CLIX which searches such databases as CCDB for small molecules which can be oriented in a binding pocket or site in a way that is both sterically acceptable and has a high likelihood of achieving favorable chemical interactions between the candidate molecule and the surrounding amino acid residues. The method is based on characterizing a binding pocket in terms of an ensemble of favorable binding positions for different chemical groups and then searching for

orientations of the candidate molecules that cause maximum spatial coincidence of individual candidate chemical groups with members of the ensemble. The current availability of computer power dictates that a computer-based search for novel ligands follows a breadth-first strategy. A breadth-first strategy aims to reduce progressively the size of the potential candidate search space by the application of increasingly stringent criteria, as opposed to a depth-first strategy wherein a maximally detailed analysis of one candidate is performed before proceeding to the next. CLIX conforms to this strategy in that its analysis of binding is rudimentary -it seeks to satisfy the necessary conditions of steric fit and of having individual groups in "correct" places for bonding, without imposing the sufficient condition that favorable bonding interactions actually occur. A ranked "shortlist" of molecules, in their favored orientations, is produced which can then be examined on a molecule-by-molecule basis, using computer graphics and more sophisticated molecular modeling techniques. CLIX is also capable of suggesting changes to the substituent chemical groups of the candidate molecules that might enhance binding.

The algorithmic details of CLIX is described in Lawrence et al. (1992) *Proteins* 12:31-41, and the CLIX algorithm can be summarized as follows. The GRID program is used to determine discrete favorable interaction positions (termed target sites) in the binding pocket or site of the protein for a wide variety of representative chemical groups. For each candidate ligand in the CCDB an exhaustive attempt is made to make coincident, in a spatial sense in the binding site of the protein, a pair of the candidate's substituent chemical groups with a pair of corresponding favorable interaction sites proposed by GRID. All possible combinations of pairs of ligand groups with pairs of GRID sites are considered during this procedure. Upon locating such coincidence, the program rotates the candidate ligand about the two pairs of groups and checks for steric hindrance and coincidence of other candidate atomic groups with appropriate target sites. Particular candidate/orientation combinations that are good geometric fits in the binding site and show sufficient coincidence of atomic groups with GRID sites are retained.

Consistent with the breadth-first strategy, this approach involves simplifying assumptions. Rigid protein and small molecule geometry is maintained throughout. As a first approximation rigid geometry is acceptable as the energy minimized coordinates of a deduced structure, describe an energy minimum for the molecule, albeit a local one. If the surface residues of the site of interest are not involved in crystal contacts then the crystal configuration of those residues is used merely as a starting point for energy minimization, and potential solution structures for those residues determined. The deduced structure should reasonably mimic the mean solution configuration.

A further assumption implicit in CLIX is that the potential ligand, when introduced into the binding pocket or site of a receptor, does not induce change in the protein's stereochemistry or partial charge distribution and so alter the basis on which the GRID interaction energy maps were computed. It must also be stressed that the interaction sites predicted by GRID are used in a positional and type sense only, i.e., when a candidate atomic group is placed at a site predicted as favorable by GRID, no check is made to ensure that the bond geometry, the state of protonation, or the partial charge distribution favors a strong interaction between the protein and that group. Such detailed analysis should form part of more advanced modeling of candidates identified in the CLIX shortlist.

Yet another embodiment of a computer-assisted molecular design method for identifying ligands of a binding pocket of the invention comprises the *de novo* synthesis of potential ligands by algorithmic connection of small molecular fragments that will exhibit the desired structural and electrostatic complementarity with an active site or binding pocket of the receptor. The methodology employs a large template set of small molecules which are iteratively pieced together in a model of a binding pocket. Each stage of ligand growth is evaluated according to a molecular mechanics-based energy function, which considers van der Waals and coulombic interactions, internal strain energy of the lengthening ligand, and desolvation of both ligand and receptor. The search space can be managed by use of a data tree that is kept under control by pruning according to the binding criteria.

In an illustrative embodiment, the search space is limited to consider only amino acids and amino acid analogs as the molecular building blocks. Such a methodology generally employs a large template set of amino acid conformations, though need not be restricted to just the 20 natural amino acids, as it can easily be extended to include other related fragments of interest to the medicinal chemist, e.g. amino acid analogs. The putative ligands that result from this construction method are peptides and peptide-like compounds rather than the small organic molecules that are typically the goal of drug design research. The appeal of the peptide building approach is not that peptides are preferable to organics as potential pharmaceutical agents, but rather that: (1) they can be generated relatively rapidly *de novo*; (2) their energetics can be studied by well-parameterized force field methods; (3) they are much easier to synthesize than are most organics; and (4) they can be used in a variety of ways, for peptidomimetic ligand design, protein-protein binding studies, and even as shape templates in the more commonly used 3D organic database search approach described above.

Such a *de novo* peptide design method has been incorporated in a software package called GROW (Moon et al. (1991) *Proteins* 11:314-328). In a typical design session, standard interactive graphical modeling methods are employed to define the structural environment in which GROW is to operate. For instance, environment could be an active site binding pocket of an F-box protein, or it could be a set of features on the protein's surface to which the user wishes to bind a peptide-like molecule. The GROW program then operates to generate a set of potential ligand molecules. Interactive modeling methods then come into play again, for examination of the resulting molecules, and for selection of one or more of them for further refinement.

To illustrate, GROW operates on an atomic coordinate file generated by the user in the interactive modeling session, such as the coordinates provided in Table 4, or the coordinates of a binding pocket or active site as described in Tables 2 and 4 plus a small fragment (e.g., an acetyl group) positioned in the active site to provide a starting point for peptide growth. These are referred to as "site" atoms and "seed" atoms, respectively. A second file provided by the user contains a number of control parameters to guide the peptide growth (Moon et al. (1991) *Proteins* 11:314-328).

The operation of the GROW algorithm is conceptually fairly simple. GROW proceeds in an iterative fashion, to systematically attach to the seed fragment each amino acid template in a large preconstructed library of amino acid conformations. When a template has been attached, it is scored for goodness-of-fit to the receptor site or

binding pocket, and then the next template in the library is attached to the seed. After all the templates have been tested, only the highest scoring ones are retained for the next level of growth. This procedure is repeated for the second growth level; each library template is attached in turn to each of the bonded seed/amino acid molecules that were retained from the first step, and then scored. Again, only the best of the bonded seed/dipeptide molecules that result are retained for the third level of growth. The growth of peptides can proceed in the N-to-C direction only, the reverse direction only, or in alternating directions, depending on the initial control specifications supplied by the user. Successive growth levels therefore generate peptides that are lengthened by one residue. The procedure terminates when the user-defined peptide length has been reached, at which point the user can select from the constructed peptides those to be studied further. The resulting data provided by the GROW procedure includes not only residue sequences and scores, but also atomic coordinates of the peptides, related directly to the coordinate system of the binding site atoms.

In yet another embodiment, potential pharmacophoric compounds can be determined using a method based on an energy minimization-quenched molecular dynamics algorithm for determining energetically favorable positions of functional groups in the binding pockets of the invention. The method can aid in the design of molecules that incorporate such functional groups by modification of known ligands or *de novo* construction.

For example, the multiple copy simultaneous search method (MCSS) described by Miranker et al. (1991) *Proteins* 11: 29-34 may be employed. To determine and characterize a local minima of a functional group in the forcefield of the protein, multiple copies of selected functional groups are first distributed in a binding pocket of interest on the F-box protein. Energy minimization of these copies by molecular mechanics or quenched dynamics yields the distinct local minima. The neighborhood of these minima can then be explored by a grid search or by constrained minimization. In one embodiment, the MCSS method uses the classical time dependent Hartree (TDH) approximation to simultaneously minimize or quench many identical groups in the forcefield of the protein.

Implementation of the MCSS algorithm requires a choice of functional groups and a molecular mechanics model for each of them. Groups must be simple enough to be easily characterized and manipulated (3-6 atoms, few or no dihedral degrees of freedom), yet complex enough to approximate the steric and electrostatic interactions that the functional group would have in binding to the pocket or site of interest in the F-box protein. A preferred set is, for example, one in which most organic molecules can be described as a collection of such groups (*Patai's Guide to the Chemistry of Functional Groups*, ed. S. Patai (New York: John Wiley, and Sons, (1989)). This includes fragments such as acetonitrile, methanol, acetate, methyl ammonium, dimethyl ether, methane, and acetaldehyde.

Determination of the local energy minima in the binding pocket or site requires that many starting positions be sampled. This can be achieved by distributing, for example, 1,000-5,000 groups at random inside a sphere centered on the binding site; only the space not occupied by the protein needs to be considered. If the interaction energy of a particular group at a certain location with the protein is more positive than a given cut-off (e.g. 5.0 kcal/mole) the group is discarded from that site. Given the set of starting positions, all the fragments are minimized simultaneously by use of the TDH approximation (Elber et al. (1990) *J Am Chem Soc* 112: 9161-9175). In this method, the forces on

each fragment consist of its internal forces and those due to the protein. The essential element of this method is that the interactions between the fragments are omitted and the forces on the protein are normalized to those due to a single fragment. In this way simultaneous minimization or dynamics of any number of functional groups in the field of a single protein can be performed.

Minimization is performed successively on subsets of, for example 100, of the randomly placed groups. After a certain number of step intervals, such as 1,000 intervals, the results can be examined to eliminate groups converging to the same minimum. This process is repeated until minimization is complete (e.g. RMS gradient of 0.01 kcal/mole/C). Thus the resulting energy minimized set of molecules comprises what amounts to a set of disconnected fragments in three dimensions representing potential pharmacophores.

The next step then is to connect the pharmacophoric pieces with spacers assembled from small chemical entities (atoms, chains, or ring moieties). In a preferred embodiment, each of the disconnected can be linked in space to generate a single molecule using such computer programs as, for example, NEWLEAD (Tschinke et al. (1993) *J Med Chem* 36: 3863,3870). The procedure adopted by NEWLEAD executes the following sequence of commands: (1) connect two isolated moieties, (2) retain the intermediate solutions for further processing, (3) repeat the above steps for each of the intermediate solutions until no disconnected units are found, and (4) output the final solutions, each of which is a single molecule. Such a program can use for example, three types of spacers: library spacers, single-atom spacers, and fuse-ring spacers. The library spacers are optimized structures of small molecules such as ethylene, benzene and methylamide. The output produced by programs such as NEWLEAD consist of a set of molecules containing the original fragments now connected by spacers. The atoms belonging to the input fragments maintain their original orientations in space. The molecules are chemically plausible because of the simple makeup of the spacers and functional groups, and energetically acceptable because of the rejection of solutions with van-der Waals radii violations.

Compounds and entities (e.g. ligands) of F-box proteins, in particular cdc4 proteins, or SCF complexes identified using the above-described methods may be prepared using methods described in standard reference sources utilized by those skilled in the art. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, New York, McGraw Hill.

Test compounds and ligands which are identified using a crystal or model of the present invention can be screened in assays such as those well known in the art. Screening may be for example *in vitro*, in cell culture, and/or *in vivo*. Biological screening assays preferably centre on activity-based response models, binding assays (which measure how well a compound binds to a binding pocket of a receptor), and bacterial, yeast, and animal cell lines (which measure the biological effect of a compound in a cell). The assays may be automated for high throughput screening in which large numbers of compounds can be tested to identify compounds with the desired activity. The biological assay may also be an assay for the binding activity of a compound that selectively binds to the binding pocket compared to other receptors.

LIGANDS/COMPOUNDS IDENTIFIED BY SCREENING METHODS

The present invention provides a ligand or compound identified by a screening method of the present invention. A ligand or compound may have been designed rationally by using a model according to the present invention. A ligand or compound identified using the screening methods of the invention may specifically associate with a target compound, or part thereof (e.g. a binding pocket). In the present invention the target compound may be the F-box protein or SCF complex or part thereof, or a molecule that is capable of associating with an F-box protein or SCF complex or part thereof (for example a substrate).

A ligand or compound identified using a screening method of the invention may act as a “modulator”, i.e. a compound which affects the activity of an F-box protein or SCF complex. A modulator may reduce, enhance or alter the biological function of an F-box protein or an SCF E3 ubiquitin ligase. For example a modulator may modulate the capacity of the F-box protein or an SCF E3 ubiquitin ligase to interact with its substrate. An alteration in biological function may be characterised by a change in specificity. For example, a modulator may cause the F-box protein to interact with a different substrate. In order to exert its function, the modulator commonly binds to a binding pocket.

A “modulator” which is capable of reducing the biological function of the enzyme may also be known as an inhibitor. Preferably an inhibitor reduces or blocks the capacity of the F-box protein or an SCF E3 ubiquitin ligase to interact with its substrate thus reducing or blocking ubiquitination of the substrate. The inhibitor may mimic the binding of a substrate, for example, it may be a substrate analogue. A substrate analogue may be designed by considering the interactions between the substrate and the F-box protein or an SCF E3 ubiquitin ligase (for example, by using information derivable from the crystal of the invention) and specifically altering one or more groups (as described above).

The present invention also provides a method for modulating the activity of an F-box protein, in particular a cdc4 protein, using a modulator according to the present invention. The invention also provides a method for modulating (e.g. potentiating or inhibiting) ubiquitination of a substrate by an SCF E3 ubiquitin ligase, by potentiating or inhibiting the substrate binding pocket of the ligase. Inhibition of ubiquitination of a substrate may decrease signaling and inhibit cellular processes that may be involved in disease. It would be possible to monitor cellular processes following such treatments by a number of methods known in the art.

A modulator may be an agonist, partial agonist, partial inverse agonist or antagonist of an F-box protein.

As mentioned above, a substrate or an identified ligand may act as a ligand model (for example, a template) for the development of other compounds. A modulator may be a mimetic of a substrate or ligand.

Like the test compound (see above) a modulator may be one or a variety of different sorts of molecule. (See examples herein.) A modulator may be an endogenous physiological compound, or it may be a natural or synthetic compound. The term “modulator” also refers to a chemically modified ligand or substrate.

The technique suitable for preparing a modulator will depend on its chemical nature. For example, peptides can be synthesized by solid phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 431 A Peptide Synthesizer (Perkin Elmer) in accordance with

the instructions provided by the manufacturer. Once cleaved from the resin, the peptide may be purified by preparative high performance liquid chromatography (e.g., Creighton (1983) *Proteins Structures and Molecular Principles*, WH Freeman and Co, New York NY). The composition of the synthetic peptides may be confirmed by amino acid analysis or sequencing (e.g., the Edman degradation procedure; Creighton, *supra*).

5 If a modulator is a nucleotide, or a polypeptide expressible therefrom, it may be synthesized, in whole or in part, using chemical methods well known in the art (see Caruthers MH *et al* (1980) *Nuc Acids Res Symp Ser* 215-23, Horn T *et al* (1980) *Nuc Acids Res Symp Ser* 225-232), or it may be prepared using recombinant techniques well known in the art.

Organic compounds may be prepared by organic synthetic methods described in references such as March,
10 1994, *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, New York, McGraw Hill.

The invention also relates to classes of modulators of F-box proteins, in particular cdc4 proteins based on the structure and shape of a substrate or component thereof, defined in relation to the substrate's spatial association with a crystal structure of the invention or part thereof.

A class of modulators may comprise a compound containing a structure of a CPD motif. In particular, the
15 modulators can comprise a CPD motif having the structural coordinates of the CPD motif in the active site binding pocket of an F-box protein. In an embodiment, a modulator comprises the structural coordinates of a CPD motif having the structural coordinates listed in Table 6.

The invention contemplates all optical isomers and racemic forms of the modulators of the invention.

PHARMACEUTICAL COMPOSITION

20 The present invention also provides for the use of a modulator according to the invention, in the manufacture of a medicament to treat and/or prevent a disease in a mammalian patient. There is also provided a pharmaceutical composition comprising such a modulator and a method of treating and/or preventing a disease comprising the step of administering such a modulator or pharmaceutical composition to a subject, preferably a mammalian patient.

The pharmaceutical compositions may be for human or animal usage in human and veterinary medicine and
25 will typically comprise a pharmaceutically acceptable carrier, diluent, excipient, adjuvant or combination thereof.

Acceptable carriers or diluents for therapeutic use are well known in the pharmaceutical art, and are described, for example, in Remington's *Pharmaceutical Sciences*, Mack Publishing Co. (A. R. Gennaro edit. 1985). The choice of pharmaceutical carrier, excipient or diluent can be selected with regard to the intended route of administration and standard pharmaceutical practice. The pharmaceutical compositions may comprise as - or in
30 addition to - the carrier, excipient or diluent any suitable binder(s), lubricant(s), suspending agent(s), coating agent(s), solubilising agent(s).

Preservatives, stabilizers, dyes and even flavouring agents may be provided in the pharmaceutical composition. Examples of preservatives include sodium benzoate, sorbic acid and esters of p-hydroxybenzoic acid. Antioxidants and suspending agents may also be used.

The routes for administration (delivery) include, but are not limited to, one or more of: oral (e.g. as a tablet, capsule, or as an ingestible solution), topical, mucosal (e.g. as a nasal spray or aerosol for inhalation), nasal, parenteral (e.g. by an injectable form), gastrointestinal, intraspinal, intraperitoneal, intramuscular, intravenous, intrauterine, intraocular, intradermal, intracranial, intratracheal, intravaginal, intracerebroventricular, intracerebral, subcutaneous, ophthalmic (including intravitreal or intracameral), transdermal, rectal, buccal, vaginal, epidural, sublingual.

Where the pharmaceutical composition is to be delivered mucosally through the gastrointestinal mucosa, it should be able to remain stable during transit through the gastrointestinal tract; for example, it should be resistant to proteolytic degradation, stable at acid pH and resistant to the detergent effects of bile.

Where appropriate, the pharmaceutical compositions can be administered by inhalation, in the form of a suppository or pessary, topically in the form of a lotion, gel, hydrogel, solution, cream, ointment or dusting powder, by use of a skin patch, orally in the form of tablets containing excipients such as starch or lactose or chalk, or in capsules or ovules either alone or in admixture with excipients, or in the form of elixirs, solutions or suspensions containing flavouring or colouring agents, or they can be injected parenterally, for example intravenously, intramuscularly or subcutaneously. For parenteral administration, the compositions may be best used in the form of a sterile aqueous solution which may contain other substances, for example enough salts or monosaccharides to make the solution isotonic with blood. The aqueous solutions should be suitably buffered (preferably to a pH of from 3 to 9), if necessary. The preparation of suitable parenteral formulations under sterile conditions is readily accomplished by standard pharmaceutical techniques well-known to those skilled in the art.

If the agent of the present invention is administered parenterally, then examples of such administration include one or more of: intravenously, intra-arterially, intraperitoneally, intrathecally, intraventricularly, intraurethrally, intrasternally, intracranially, intramuscularly or subcutaneously administering the agent; and/or by using infusion techniques.

For buccal or sublingual administration the compositions may be administered in the form of tablets or lozenges which can be formulated in a conventional manner.

The tablets may contain excipients such as microcrystalline cellulose, lactose, sodium citrate, calcium carbonate, dibasic calcium phosphate and glycine, disintegrants such as starch (preferably corn, potato or tapioca starch), sodium starch glycollate, croscarmellose sodium and certain complex silicates, and granulation binders such as polyvinylpyrrolidone, hydroxypropylmethylcellulose (HPMC), hydroxypropylcellulose (HPC), sucrose, gelatin and acacia. Additionally, lubricating agents such as magnesium stearate, stearic acid, glyceryl behenate and talc may be included.

Solid compositions of a similar type may also be employed as fillers in gelatin capsules. Preferred excipients in this regard include lactose, starch, cellulose, milk sugar or high molecular weight polyethylene glycols. For aqueous suspensions and/or elixirs, the agent may be combined with various sweetening or flavouring agents,

colouring matter or dyes, with emulsifying and/or suspending agents and with diluents such as water, ethanol, propylene glycol and glycerin, and combinations thereof.

As indicated, a therapeutic agent (e.g. modulator) of the present invention can be administered intranasally or by inhalation and is conveniently delivered in the form of a dry powder inhaler or an aerosol spray presentation from a pressurised container, pump, spray or nebuliser with the use of a suitable propellant, e.g. dichlorodifluoromethane, trichlorofluoromethane, dichlorotetrafluoroethane, a hydrofluoroalkane such as 1,1,1,2-tetrafluoroethane (HFA 134ATM) or 1,1,1,2,3,3,3-heptafluoropropane (HFA 227EATM), carbon dioxide or other suitable gas. In the case of a pressurised aerosol, the dosage unit may be determined by providing a valve to deliver a metered amount. The pressurised container, pump, spray or nebuliser may contain a solution or suspension of the active compound, e.g. using a mixture of ethanol and the propellant as the solvent, which may additionally contain a lubricant, e.g. sorbitan trioleate. Capsules and cartridges (made, for example, from gelatin) for use in an inhaler or insufflator may be formulated to contain a powder mix of the agent and a suitable powder base such as lactose or starch.

Therapeutic administration of polypeptide modulators may also be accomplished using gene therapy. A nucleic acid including a promoter operatively linked to a heterologous polypeptide may be used to produce high-level expression of the polypeptide in cells transfected with the nucleic acid. DNA or isolated nucleic acids may be introduced into cells of a subject by conventional nucleic acid delivery systems. Suitable delivery systems include liposomes, naked DNA, and receptor-mediated delivery systems, and viral vectors such as retroviruses, herpes viruses, and adenoviruses.

APPLICATIONS

The invention further provides a method of treating a mammal, the method comprising administering to a mammal a modulator or pharmaceutical composition of the present invention.

In particular, the invention contemplates a method of treating or preventing a condition or disease associated with an F-box protein or SCF complex in a cellular organism, comprising:

- (a) administering a modulator of the invention in an acceptable pharmaceutical preparation; and
- (b) activating or inhibiting an F-box protein or SCF complex or their interaction with a substrate to treat or prevent the disease.

The invention provides for the use of a modulator identified by the methods of the invention in the preparation of a medicament to treat or prevent a disease in a cellular organism. Use of modulators of the invention to manufacture a medicament is also provided.

Typically, a physician will determine the actual dosage of a modulator or pharmaceutical composition of the invention that will be most suitable for an individual subject and it will vary with the age, weight and response of the particular patient and severity of the condition. There can, of course, be individual instances where higher or lower dosage ranges are merited.

The specific dose level and frequency of dosage for any particular patient may be varied and will depend upon a variety of factors including the activity of the specific compound employed, the metabolic stability and length of action of that compound, the age, body weight, general health, sex, diet, mode and time of administration, rate of

excretion, drug combination, the severity of the particular condition, and the individual undergoing therapy. By way of example, the pharmaceutical composition of the present invention may be administered in accordance with a regimen of 1 to 10 times per day, such as once or twice per day.

For oral and parenteral administration to human patients, the daily dosage level of the agent may be in single or divided doses.

The modulators and compositions of the invention may be useful in the prevention and treatment of conditions involving aberrant F-box proteins or SCF complexes. In particular the modulators and compositions may be useful in treating cancer or Alzheimer's Disease.

Conditions which may be prevented or treated in accordance with the invention include but are not limited to lymphoproliferative conditions, and malignant and pre-malignant conditions. Malignant and pre-malignant conditions may include solid tumors, B cell lymphomas, chronic lymphocytic leukemia, chronic myelogenous leukemia, prostate hypertrophy, Hirschsprung disease, glioblastoma, breast and ovarian cancer, adenocarcinoma of the salivary gland, premyelocytic leukemia, prostate cancer, multiple endocrine neoplasia type IIA and IIB, medullary thyroid carcinoma, papillary carcinoma, papillary renal carcinoma, hepatocellular carcinoma, gastrointestinal stromal tumors, sporadic mastocytosis, acute myeloid leukemia, large cell lymphoma or Alk lymphoma, chronic myeloid leukemia, hematological /solid tumors, papillary thyroid carcinoma, stem cell leukemia/lymphoma syndrome, acute myelogenous leukemia, osteosarcoma, multiple myeloma, preneoplastic liver foci, and resistance to chemotherapy.

Modulators and compositions of the invention may be used to restore function to a mutant F-box protein, in particular a mutant cdc4 polypeptide. Modulators and compositions of the invention, in particular inhibitors may also have utility in treating diseases associated with F-box mutations, in particular cdc4 polypeptide mutations, in combination with other cancer mutations, Notch pathway mutations or presenilin mutations.

A modulator of the invention may be used to promote binding of a substrate to a SCF complex. In an embodiment a modulator that associates (preferably with high affinity) with a binding pocket of a SCF complex as described herein, is linked to an agent that binds to a substrate to be ubiquitinated by a SCF complex. A modulator-agent-substrate complex where the modulator is derived from a binding pocket of an F-box protein as described herein may be used in treating diseases associated with a mutant F-box protein.

Therapeutic efficacy and toxicity of compositions and modulators of the invention may be determined by standard pharmaceutical procedures in cell cultures or with experimental animals, such as by calculating the ED_{50} (the dose therapeutically effective in 50% of the population) or LD_{50} (the dose lethal to 50% of the population) statistics. The therapeutic index is the dose ratio of therapeutic to toxic effects and it can be expressed as the ED_{50}/LD_{50} ratio. Pharmaceutical compositions that exhibit large therapeutic indices are preferred.

The invention will now be illustrated by the following non-limiting examples:

EXAMPLE 1

The following methods were used in the investigation described in the example:

Methods

Cloning, Protein expression and Purification

The Cdc4 fragment employed for crystalization, which is deleted for terminal residues 1 to 262 and 745 to 779, extends from the beginning of the F-box domain to the end of the WD40 repeat domain. The N-terminal deletion removes a poorly conserved sequence of 226 amino acids and a conserved element of approximately 40 residues termed the D-domain that immediately precedes the fbox domain and that has been implicated in molecular multimerization. The C terminal deletion removes residues not conserved amongst different Cdc4 homologues. Both Skp1 and Cdc4 were engineered to remove flexible loops, namely residues 36-55 in Skp1 and residues 601 to 604 and 609 to 624 in Cdc4.

A PCR product containing CDC4(263-744) was cloned into the *EheI*(SfoI) and *Bam*H1 sites of pPROEX HTb. In parallel, a PCR product containing SKP1 Δ 37-64 was cloned into the *NdeI* and *Bam*HI sites of pGEX2T-TEV. An *SspI* GST-SKP1-containing fragment from this construct was cloned into the *StuI* site of the Cdc4 construct described above such that CDC4 and SKP1 were in opposite orientations. A non-homologous region in CDC4 encoding amino acids 602-624 was then replaced by the DNA sequence GGCGAACTG [SEQ ID NO. 39], which encodes the shorter peptide sequence Gly-Glu-Leu.

The Cdc4/skp1 complex was expressed in *E. coli* B934 (DE3) cells grown in minimal media supplemented with a mixture of selenomethionine (40 ug/ml) and methionine (0.4ug/ml). Cells were induced with 0.2 mM isopropyl- β -D-thiogalactopyranoside (IPTG) at 15° C overnight. Cell pellets were resuspended in 50 mM hepes pH 7.5, 500 mM NaCl , 10% glycerol, and 5 mM Imidazole, lysed with a cell homogenizer (Emulsiflex C-5, Avistin) followed by a 20 sec sonication (vibra cell, Betatec). The lysate was then clarified by centrifugation at 65 000 x g for 40 min. The supernatant was loaded onto a 5 ml metal chelating column (Pharmacia) and eluted in high imidazole. This fraction was loaded onto a glutathione-sepharose column (Pharmacia) and the bound complex was eluted by overnight digestion with TEV protease (Canadian Life). Eluted protein was dialysed to remove DTT and EDTA and reloaded onto a metal chelating column. The flow through containing the complex was concentrated and applied to a Superdex S 75 gel filtration column (Pharmacia). Fractions containing the complex were concentrated in a buffer containing 10 mM hepes pH 7.5, 250 mM NaCl, and 1 m M DTT.

Crystallization, Data Collection, and Structure Determination

Hanging drops containing 1 μ l of 21 mg/ml protein plus 1.2 molar equivalents of the CPD peptide sequence were mixed with equal volumes of reservoir buffer containing 0.1 M Tris pH 8.5, and 1.5 M ammonium sulphate. Crystals were flash frozen in reservoir buffer supplemented with 15% glycerol. Crystals of the space group P3₂, (a = 107.7Å, b = 107.7Å, c = 168.3Å, α = γ = 90°, β = 120°), with two molecules of the complex in the asymmetric unit were obtained at 20°C. A Multiple Anomalous Dispersion (MAD) experiment was performed on a frozen crystal at the Advanced Photon Source (Argonne, IL) (APS) beamline BM 14-B and BM 14-D(λ 1 = 0.9798 Å, λ 2 = 0.9800 Å, λ 3 = 0.9000 Å) using a Quantum 4 ADSC CCD detector. Data processing and reduction was carried out with the HKL program suite (Otwinowski and Minor, 1997). The programs SHARP (de La Fortelle and Bricogne, 1997) and

SnB (Miller et al., 1994) were used in combination to locate and refine 19 of the 22 Se sites. Following density modification with Solomon (Abrahams and Leslie, 1996), a partial model was generated using O (Jones et al., 1991) and refined using CNS (Brunger et al., 1998) to a working R value of 24.09% and a free R value of 28.71%. Pertinent statistics for data collection and refinement are shown in Table 1.

The increased order of the second CPDs may be due to a crystal packing interaction involving the c-terminus of the CPD. While the main chain termini of the second CPD are discernable (Figure 3e), the precise backbone and side chain conformations for the P-2 Leu, P-3 Gly, P+4 Ser, and P+5 Gly are less reliably determined.

Mutagenesis

Point mutants were obtained by a PCR-based approach using oligos provided in supplementary information and Pfu polymerase (Stratagene). Once verified by sequencing the mutants were sub-cloned into the appropriate vectors as listed in the supplementary information. Alanine insertion mutations were obtained using the Kunkel method (ref) and then sub-cloned into the vectors indicated in the supplementary information.

Shuffle experiments

All mutants on a TRP1 ARS CEN plasmid were transformed into a *cdc4Δ* strain (MT 1259) containing a wildtype copy of CDC4 on a URA3 ARS CEN plasmid. Cells were plated on either Trp⁻ Ura⁻ or 5-FOA medium for 2 days at 30° C. Viable cells on 5-FOA were grown in Trp⁻ medium and transformed with either wild type GAL1-SIC1, GAL1-SIC T45A, or GAL1-SIC T33V on a LEU2 ARS CEN pasmid . Cells were then plated on Leu- Trp- plates containing either glucose or galactose and incubated for 2 days at 30° C.

Sic1-Cdc4 interactions.

Bacterially expressed His6-Sic1 was phosphorylated with Cln2-Cdc28 kinase purified from baculovirus infected Sf9 cells as described before (Nature paper). 1ug of WT or mutant Cdc4-GST-Skp1, immobilized on GSH-Sepharose resin, was incubated with 0.5ug phospho-Sic1 at 4C for 1h and washed 4 times. Captured complexes were resolved on SDS-PAGE and Sic1 visualized by anti-Sic1 Western blotting and ECL. For IEF-2D analysis, several Sic1 phosphorylation reactions were carried out for different time periods to obtain a spectrum of Sic1 that were phosphorylated at different numbers of its nine CDK sites. This pool of phospho-Sic1 (2.5ug) was incubated with 5μg of WT or mutant Cdc4-GST-Skp1 as described above. Different phosphorylation states of Sic1 were separated by denaturing isoelectric focusing (IEF)-2D gel electrophoresis and visualized by anti-Sic1 Western blotting and ECL. IEF was performed using pH3-10NL Immobiline gel strips and IPGphor IEF system (Amersham pharmacia).

Results

The x-ray crystal structure presented herein consists of a ternary complex of yeast Skp1 bound to a fragment of Cdc4, and a 9mer high affinity CPD phosphopeptide (Figure 2). The Cdc4 fragment, which is deleted for terminal residues 1 to 262 and 745 to 779, extends from the beginning of the F-box domain to the end of the WD40 repeat domain.

Skp1- Cdc4 Fbox: Skp1 forms an elongated structure with a mixed α/β topology identical to that reported for human Skp1 (Schulman et al, 2000). The topology consists of a three-strand (denoted $\beta 1$ to $\beta 3$) β -sheet and eight α -helices,

denoted $\alpha 1$ to $\alpha 8$ (Figure 2a). The structure of Cdc4 from its amino terminus consists of an F-box domain, an α -helical extension or linker, and a WD40 repeat domain (Figure 2a,b). The F-box domain comprises five α helices (denoted $\alpha 0$ to $\alpha 4$). This topology differs slightly from that reported for the F-box domain of hSkp2 (Schulman et al, 2000), which consists of a loop region L1 and three helices denoted $\alpha 1$ to $\alpha 3$. Helix $\alpha 0$ in Cdc4 corresponds most closely in sequence and position to the loop region L1 of Skp2 while a half turn remnant of helix $\alpha 4$ is discernable in the transition sequence between the Skp2 F-box and Leucine Repeat domains. As observed in the Skp1-Skp2 complex, Skp1 and the F-box domain of Cdc4 associate by the interdigitation of helices $\alpha 0$ to $\alpha 3$ of Cdc4 with helices $\alpha 5$ to $\alpha 8$ of Skp1. This mode of inter-domain association is characterized by a common and continuous hydrophobic core that spans the two protein domains.

Cdc4 helical linker and WD40 domain: Following the F-box domain of Cdc4 is a helical extension that forms a structured bridge to the WD40 repeat domain. The helical extension consists of two α -helices $\alpha 5$ and $\alpha 6$ that together with helices $\alpha 3$ and $\alpha 4$ of the F-box domain form a stalk and pedestal like structure that connects and orients the WD40 domain (Figure 2c).

Eight copies of the WD40 repeat motif in Cdc4 form an 8 blade β -propeller structure. Each blade, composed of 4 anti-parallel β -strands, is related by 8-fold pseudo symmetry about a central axis (Figure 2b). As first shown for G-protein gamma subunit (Sondek 1996), the WD40 repeat motif of approximately 40 amino acids composes the outer β -strand of one propeller blade and the inner three strands of the adjacent blade. A continuous circular arrangement of blades is formed by the association of the first and last WD40 repeat motifs to form the 8th propeller blade. Interestingly, a 7 β -propeller blade structure was anticipated for Cdc4 and its orthologues (and generally all WD40 repeat F-box adaptors), which is attributable in part to the cryptic nature of the 8th WD40 repeat motif (Figure 1). Based on the structure based sequence alignment in Figure 1, it is predicted that the other WD40 class of F-box adaptor proteins (i.e. the Met30 orthologues and β TRCP orthologues) will form 7-blade β -propeller structures.

The WD40 repeat domain forms a disk like structure characterized by a cavity in the middle and two opposing circular surfaces of slightly different size. The smaller of the two surfaces composes the CPD binding site. On the bottom surface is anchored helix $\alpha 6$ of the helical extension, which inserts obliquely between propeller blades $\beta 7$ and $\beta 8$. Interestingly, β -propeller blade 2 consists of 5 β -strands. The outermost strand of this blade, denoted $\beta 9^1$, is non-standard and arises from an amino acid insert in the connecting loop between β -strands 12 and 13. Strand $\beta 9^1$ forms a parallel arrangement with strand $\beta 9$, which differs from the anti parallel architecture of all other β -strand elements in the WD40 domain structure. A large insert in the $\beta 12$ - $\beta 13$ linker is absent from dr, ce, hu, mu Cdc4 homologues suggesting that a 5 β -strand propeller blade 2 is unique to the fungal homologues.

A fixed orientation between the F-box domain and WD40 domain of Cdc4 is maintained largely through the integrity of the stalk like helix $\alpha 6$ of the helical extension (Figure 2c). Helix $\alpha 6$ is 30Å in length, and is anchored at its N-terminus to the hydrophobic core of the F-box/helical extension and at its C-terminus to the hydrophobic core of

the WD40 repeat domain. In contrast to the intermolecular connection between Skp1 and the F-box domain, the connection between the F-box domain and WD40 repeat domain appears less rigidly structured.

At its amino terminus, helix $\alpha 6$ anchors to the F-box through hydrophobic interactions involving $\alpha 6$ residues Phe 355 and Leu 356 and F-box residues Ile 295, and Ile 296, Leu 315, Trp 316, and Leu 319 (Figure 2c). Helix $\alpha 5$ packs along side the base of helix $\alpha 6$ opposite to the F-box domain through hydrophobic packing interactions involving Tyr342, Leu 338 and Leu 334. At its C- terminus, helix $\alpha 6$ anchors through hydrophobic interactions involving residues Trp 365 and Ile 364 with WD repeat residues Val 687, Ile 696, Leu 726 and Phe 743 in β -propeller blades 7 and 8. Asn 364 of helix $\alpha 6$ also forms a tight hydrogen bond interaction with the backbone carbonyl group of Phe 743 in propeller blade 8. The noted interactions (with the exception of interactions involving helix $\alpha 5$) involve residues that are conserved across most WD40 F-box adaptor proteins including the Met30 orthologues and β -TRCP orthologues, which suggests that the linkage between WD40 and F-box domains are similarly structured in these proteins. Helix $\alpha 6$ in β -TRCP, however, appears to be one α -helical turn longer (Figure 1).

Outside of stalk helix $\alpha 6$, only two close contacts ($< 3.5\text{\AA}$) are observed between the WD40 repeat domain and other regions of Cdc4. These contacts consist of hydrogen bonds between Asn684 and Arg700 in the loop regions of propeller blade 7 with Glu 323 in the $\alpha 4$ - $\alpha 5$ linker of the helical extension. Both, hydrogen bonds are maintained in the two Cdc4 molecules of the crystal asymmetric unit but all three residues are poorly conserved amongst Cdc4 orthologues (Figure 1). The lack of additional stabilizing interactions suggests that the F-box/WD40 domain linkage is not exceedingly rigid, and indeed, the WD40 domain in the two molecules of the asymmetric unit differ relative to their F-box domains by a 5 degree rotation about helix $\alpha 6$.

WD40 domain phosphopeptide recognition: A nine-mer CPD consisting of the sequence acetyl-Gly,Leu,Leu,pThr,Pro,Pro,Gln,Ser,Gly-amide [SEQ ID NO.40] is bound to the front face of the WD40 domain of Cdc4. In the two WD40 repeat domain/CPD complexes of the crystal asymmetric unit, a central core of 4 CPD residues corresponding to the sequence Leu, pThr, Pro, Pro [SEQ ID NO.41] is well ordered.

These residues have been modeled unambiguously in unbiased experimental electron density maps (Figure 3e). Interpretable electron density is also apparent for the P-2 Leu, P-3 Gly, P+3 Gln, P+4 Ser, and P+5Gly positions of the second CPD (no interpretable electron density is apparent for these residues in the first CPD). The CPD binds in an extended manner across β -propeller blade 2 with the N-terminus oriented towards the central cavity of the WD40 repeat domain and the C-terminus oriented towards the outer rim. The CPD binding surface of Cdc4 is composed of invariant and highly conserved residues from β -propeller blades 1 to 6 and 8 and represents the most conserved part of the WD40 repeat domain surface (Figure 3a,c).

Cdc4 displays an absolute requirement for phosphorylation at Ser or Thr at the P-0 position of the CPD. In the crystal structure, the P0 pThr phosphate group is coordinated by an intricate network of electrostatic interactions and hydrogen bonds involving residues absolutely conserved across all Cdc4 orthologues (Figure 3c). The P0 phosphate group forms direct electrostatic interactions with the guanidinium groups of Arg 485, Arg 467, and Arg 534

and a direct hydrogen bond with the side chain of Tyr 548. The side chain of Tyr 548 is coordinated by stacking interactions with the guanidinium group of Arg 572, which in turn is coordinated by a hydrogen bond to the side chain of Tyr 574. Although Cdc4 shows a strong (6 fold) preference for pThr over pSer, the structural basis for this selectivity is not obvious. In the crystal structure, the C γ methyl group of Thr is directed towards solvent and does not make contact with the CPD binding surface of Cdc4. This binding preference may be due to the greater side chain rotational stability arising from the Thr β -branch structure.

Cdc4 displays an absolute requirement for proline in the P+1 CPD position. In the crystal structure, the P+1 proline side chain projects into a three-sided pocket on the CPD binding surface. The side chain of Trp 426 forms one side of the pocket and packs in a coplanar manner with the P+1 proline side chain. On its other side, the Trp 426 side chain packs tightly against the side chain of Thr 386. The opposite side of the P+1 binding pocket is formed by the side chain of Arg 485. Arg 485 coordinates the P+1 Proline through van der Waals side chain interactions and through a direct hydrogen bond to the Proline backbone carbonyl group. This represents the sole direct hydrogen bond interaction between Cdc4 and the CPD main chain. The side chains of Thr 441 and Thr 465 define the remaining side of the P+1 Proline binding pocket, with the C γ side chain groups composing a hydrophobic surface. The hydroxyl groups of Thr 441 and 465 orient away from the P+1 binding pocket, where they are well placed to influence binding specificity for CPD residues C-terminal to the P+1 position. Unlike Trp 426, Thr 386 and Arg 485, which are invariant amongst the Cdc4 orthologues, Thr 441 and Thr 465 are substituted with Ile in the *S. pombe* Cdc4 orthologue Pop1. The modeling studies suggest that this substitution has no effect on the P+1 binding pocket but may perturb CPD binding specificity C-terminal to the P+1 positions through steric effects (Ile is bigger than Thr) and by increasing the hydrophobic character of the surface.

Cdc4 displays a strong preference for the hydrophobic residues Leu, Ile and Proline at the P-1 and P-2 CPD positions. In the crystal structure, the P-1 Leucine side-chain is oriented towards a hydrophobic pocket composed of invariant residues Trp 426, Trp 717, and Thr 386, and the conserved hydrophobic residue Val 384. While less precisely modeled, the main chain position of Leu +2 lies in close proximity to a third hydrophobic pocket composed of the invariant residue Tyr574, and the conserved hydrophobic residues Met 590 and Leu634.

Cdc4 displays little preference for residues in the P+2 to P+5 CPD positions. In the crystal structure, the side chain of P+2 Pro is directed towards solvent (which would account for the lack of selectivity at this position), while the main chain conformation of Pro +1 and Pro+2, causes the CPD to kink away from the peptide-binding surface from the Pro+2 position onwards. As a result, only one additional close contact with Cdc4 is made by the CPD following the Pro +1 position, which consists of a weak hydrogen bond (sub-optimal geometry) between the P+4 Gln side chain and the side chain of Arg 485.

Adjacent to the P+1 proline binding pocket, Ser 464, Thr 441 and Thr 465 are well placed to exert specificity for the +3 and +4 CPD positions if an extended rather than kinked conformation of the CPD were adopted. As noted, Thr 441 and 465 are substituted with Ile in the Cdc4 orthologue pop1 in *S. pombe*. While nothing is known about the

effect of this substitution on CPD recognition, it is predicted that this could have some effect on substrate selectivity for the P+2 to P+5 CPD positions.

Cdc4 displays strong selectivity against Arginine and Lysine in positions -2, -1, +2, +3 and +4. This selectivity may be due to electrostatic repulsion generated by the invariant Cdc4 residues Arginine 572, 534, 467, 485 and 443, which dominate the local electrostatic character of the CPD binding site. Lys 402 is also well placed to contribute to repulsive effects but this position is not conserved amongst the Cdc4 orthologues. The selectivity against positively charged residues in the P-2 to P-1 CPD positions can also be reconciled in part by the hydrophobic nature of the P-1 and P-2 binding pockets and indeed, oppositely charged Glu and Asp residues are also disfavored at these CPD positions.

10 Comparison with Skp1-Skp2 complex:

Skp2 is a representative member of a second class of F-box adaptor proteins, which possesses a leucine repeat domain in place of the WD40 repeat of Cdc4. In addition to providing a first structural view of a Skp1 homologue and an F-box domain, the structure of the Skp1/Skp2 complex revealed a mode of molecular association predicted to be employed by all Skp1/F-box homologues. The Cdc4/Skp1/CPD structure confirms the fold of the individual Skp1 and F-box domains and their mode of association. Superposition of yeast and human Skp1 strands $\beta 1$ - $\beta 3$ and helices $\alpha 1$ to $\alpha 7$ (RMSD C α = 0.74Å) reveals a close correspondence between F-box helices $\alpha 1$ to $\alpha 3$ with only Skp1 helix $\alpha 8$ and F-box helix $\alpha 4$ showing significant deviations between the two structures. In addition, only the first half of helix $\alpha 8$ is ordered in ySkp1 and only has a half turn fragment of the F-box helix $\alpha 4$ is apparent in Skp2. The differences in positions and lengths of F-box helices $\alpha 4$ and Skp1 helices $\alpha 8$ reflects the different roles these secondary structure elements play in the linkage between their respective F-box and ligand binding domains.

The structure of the Skp1/Skp2 complex revealed a solid/substantial linkage between its Leucine Repeat and the F-box domains, a feature predicted to be shared by all Skp2 F-box orthologues. In Skp2, the F-box domain helix $\alpha 4$ terminates abruptly and without an appreciable linker, makes an immediate transition to the Leu Repeat domain fold. This linkage is enhanced by a β -strand projecting back from C-terminus of the Leu repeat domain and helix $\alpha 8$ projecting forward from Skp1. The sum of linker region interactions compose a local hydrophobic network that links the hydrophobic cores of the F-box domain with that of the LRR domain. This contrasts sharply with the corresponding linkage of Cdc4, which is composed primarily by a lengthy inter-domain linker (the helical extension) and which lacks significant involvement of Skp1 or the WD40 repeat domain for stabilization.

Although the Skp2 and Cdc4 F-box adaptor proteins employ structurally divergent ligand binding domains, the general position of the WD40 and LRR domains are surprisingly similar. The precise ligand-binding site on Skp2 has not been determined but mutagenesis studies on the Skp2 orthologue in Met30 have mapped the ligand binding site to the inner side of the curved surface. If the Skp2 binding site is inferred from the overlap with the Cdc4 CPD binding site, the CPD site would map to the lateral side of the Leu repeat domain.

Model of the SCF^{Cdc4} E2 complex

The structure of Cdc4 bound to substrate provides a missing piece of the larger SCF structural puzzle and sheds light on how substrate is presented for ubiquitination. A complete model of the SCF^{Cdc4}-E2-substrate complex consisting of an E2, a cullin, a ring finger domain, an F-box adaptor, Skp1, and CPD has been constructed using the structures of individual component proteins and/or larger assemblies determined previously (Figure 4). Two interesting features are apparent. Firstly, a separation distance between the E2 active site cysteine and the peptide-binding site of Cdc4 is very large at 64Å and second Cdc4 presents the CPD peptide with a direct line of sight to the E2.

Mutational analysis of CPD binding surface

In order to probe the functional importance of amino acid residues on the highly conserved peptide binding surface, a panel of Cdc4 mutants (both single and double mutants) were generated and tested each for its ability to bind phospho Sic1 and Skp1 in vitro using a pull down assay and for its ability to substitute for wt-cdc4 in vivo using a cell viability assay. Of 12 single site mutants tested, only Arg 467, Arg485Ala Arg534Ala, and Trp 426 abolished both cell viability in vivo and phosphoSic1 binding in vitro. Together, these residues compose most of the interaction surface with the pThr, Pro CPD core. Interestingly, Tyr 548, the only other amino acid on the surface of CDC4 to directly contact P0 phosphate group, is functional in vivo but is compromised for CPD binding in vitro. Mutation of the adjacent residue Arg572 to Ala shows the same behavior. For the Arg572 mutation, the inability to bind psic1 in vitro appears due to its tendency to aggregation. Presumably in the context of the full SCF complex in vivo this mutant is sufficiently well behaved to bind phospho Sic1.

All other single site mutants including Arg443Ala, Lys402Ala, Tyr574Ala, Trp717, Val384, and the double site mutant Thr441/465Ile, K404D/R443D and V384N/W717N are viable when expressed in the cdc4 delete and are fully competent for phosphoSic1 binding in vitro.

Since the cell viability assay may be masking subtle functional roles for the conserved Cdc4 residues, function was assayed in vivo under more stringent conditions in which Sic1^{wt} or the stabilized mutants, Sic1(T33V) or Sic1(T45A) are over-expressed under a galactose promoter. This should amplify defects in cdc4 function. Under these conditions, Trp 717, Tyr 548 and the double mutant K404D/R443D are lethal showing that these residues are in fact important for function.

Role of the Stem and pedestal structure

To probe the role of the F-box WD40 inter-domain linker, point mutations, insertions or deletions were introduced into the stem and pedestal structure of Cdc4 and protein function was assessed as performed for the peptide binding site mutants.

Deletion of helix α5 or introduction of Proline and Glycine helix destabilizing residues within the helix had no effect on Cdc4 function both in vitro and in vivo. This result is consistent with the poorly conserved nature of helix α5 and its flanking linker regions. Helix 5 appears entirely absent from human, mouse and drosophila homologues and helix destabilizing substitutions in helix 5, incorporating glycine and proline, are observed in the

worm and fungal homologues (Figure 1). A more invasive deletion of helix 5 that deletes part of the linkers to helix 4 and helix 6 was inviable in yeast. This mutant is properly folded as evidence by the finding that the protein can bind both Skp1 and phospho Sic 1 in vitro. This mutation should likely disrupt the positioning of helix 6 relative to the fbox domain (the linker is too short to span the two secondary structure elements).

5 The introduction of helix destabilizing residues in helix $\alpha 6$ or the lengthening of the helix by the insertion of one, two, three, four, 8 or 12 amino acid residues also disrupted protein function in vivo, without while maintaining the ability of Cdc4 to bind pSic1 and Skp1. These results are consistent with a possible role for helix 6 in presenting bound substrates in a specific geometric orientation.

10 It is peculiar that such a spindly structure is sufficient to maintain rigidity. Perhaps in the context of the dimer, additional contacts help to stabilize position of the WD repeats with respect to the other part of the protein. Indeed, the N terminal dimerization domain is required for function. Or perhaps a modicum of flexibility is important for the catalytic mechanism.

Probing substrate selectivity against positively charged residues

15 Cdc4 bind Sic1 in a multi site dependent manner. Each of the phosphorylation sites in Sic1 are sub-optimal in isolation but series of 5 to 7, they work cooperatively to bind to Cdc4 through an avidity effect. Part of the sub-optimal character of the sites is due to the presence of Lysine in the +2 to +5 positions. From the crystal structure, the selectivity against positive residues appear to arise from electrostatic repulsion from highly conserved residues on the CPD binding surface of Cdc4. To test this hypothesis, two residues not directly involved in phosphopeptide binding were mutated and then the multi site requirement for phosphoSic1 binding was evaluated (Figure 5c).

20 Using an IEF pull down assay, wild type Cdc4 is shown to selectively binds to the 5,6 and 7 site phosphorylated phosphoSic1 from a pool of single to 9 site phosphorylated forms. In contrast, the double mutant binds to 3,4,5,6,7 site phosphorylated forms of Sic1 (Figure 5a). This supports the notion of selectivity and the basis for avidity that may be important for setting sensitive threshold for cell cycle progression (Figure 5b). The same effect was observed for a double mutant.

25 Cancer causing mutations in drosophila and human Cdc4

Mutations in human and fly orthologues of yCdc4 give rise to cancers (see Table below). All mis-sense mutations map to the WD40 CPD binding domain and either have been demonstrated or are predicted to perturb CPD binding function. In previous studies, two cancer cell lines tested positive for mutations at Arginine 534 and Arg 467 (Arg 534 and Arg 467 in yCdc4). In the crystal structure, these residues make a direct binding interaction with the P0 phospho group and our mutational analysis demonstrates an absolute requirement of these residues for CPD binding. 30 In another study, two endometrial cancerous tissue samples tested positive for mutations equivalent to Arg467 and Arg 485 in yCdc4. As for the tumor cell line mutations, these mutations affect key residues required for CPD recognition.

Two mutations characterized in drosophila cancer include Ala118Val and Gly1132Glu, corresponding to 35 yCdc4 positions Ser532 and Gly546 respectively. The first of these mutations, involve the substitution of a small

Ala/Ser residue with a bulkier b-branched Valine residue. This may compromise CPD binding function through steric effects on the position of Arg434, Arg467, Arg534 triad. In the crystal structure, Ala/Ser is positioned centrally amongst the triad. The second drosophila mutation, Gly1132Glu, maps to β -strand 15 of propeller blade 4 in yCdc4. This position is within the core of the protein and mutation here likely acts by disrupting the overall WD40 domain fold or through local perturbations of structure that indirectly affect the phosphate binding pocket. Glycine in this position of the WD40 repeat motif is highly conserved. The temperature sensitive alleles previously characterized including Gly398Glu in propeller blade 1 and Ser438Asn in propeller blade 2 likely act by disrupting the fold in a similar manner to disrupt the overall WD fold. These are more distantly located from the CPD binding pocket.

Cancer Mutations

H-cell lines	Drosophila	Entrometrial	Orlicky	Rosamond
Arg534(425)Leu Arg 467(385)Cys	Ser/Ala532(1118)Val Gly546(1132)Glu	Arg467(465)His Arg485(479)Gln	Arg534Ala Arg467Ala Arg485Ala Trp426Ala	Gly398Gln Ser438Asn

Discussion

Recognition of phosphorylated substrates by the ubiquitin system.

Substrate selection by Cdc4. The structure of the Skp1-Cdc4-CPD complex reveals the basis for phosphorylation-dependent recognition, the specificity of which is governed by three primary determinants. The substrate phosphothreonine is locked in place by direct contacts with three conserved and essential Arg residues. The preference for hydrophobic residues at the P-1 position (and perhaps P-2 position) is enforced by a hydrophobic pocket that lines the center of the WD40 propeller. Finally, the bias against basic residues at P+2 to P+5 is established by two conserved Arg residues positioned on the top of the propeller directly in-line with the axis of the bound peptide. These conclusions are supported by mutagenesis of key residues in Cdc4 and by structure-based engineering of Cdc4 to accept sub-optimal CPD sequences.

The construction of the Cdc4 phospho-peptide binding module differs from that of known phospho-Ser/Thr binding modules in an important respect. Known phospho-recognition domains, such as 14-3-3, WW and FHA domains appear to be composed of a series of dedicated interaction sites, each of which contributes incrementally to the overall binding interaction (Yaffe and Elia, 2001). The Cdc4-substrate interaction is dominated by extensively coordinated phospho-Thr and Pro residues, as well as by a striking positive electrostatic potential around the binding site. The hydrophobic pocket that selects residues in the P-2 and P-1 positions also contributes to binding affinity. In contrast to other phospho-recognition modules, however, the strong binding of the phosphorylated residue is partially offset by specific selection against basic residues in the substrate peptide, through electrostatic repulsion from a basic patch downstream of the phosphate binding pocket. These features allow the binding affinity for any given peptide to be precisely tuned. Thus, all of the natural CPD motifs in Sic1 are sub-optimal in one or more respects; indeed only peptides derived from the T45 site exhibit any detectable interaction with Cdc4 (Nash et al., 2001). These features

establish a requirement for substrate phosphorylation on multiple sites, which mediate a high affinity interaction in a manner that depends cooperatively on the number of phosphorylated residues.

In the case of wild type Sic1, at least six sites must be phosphorylated for high affinity binding by Cdc4. As shown here, mutation of the basic selection residues shifts the binding equilibrium to lower phosphorylated forms while in previous studies, it was demonstrated that introduction of a single optimal CPD into Sic1 causes premature Sic1 degradation and genome stability (Nash et al., 2001). An advantage of this system is that not only can the affinity of individual sites be tuned over a broad range, but the number and spacing of sites can be readily varied to establish a threshold for the targeting kinase. Thus Cdc4 is able to target numerous critical factors for phosphorylation-dependent degradation, including the Cdk inhibitor Sic1, the polarization factor Far1, the replication initiator Cdc6 and the transcription factor Gcn4, all of which may be controlled with different kinetics and different phosphorylation thresholds (Deshaies, 1999). These properties distinguish Cdc4 from other known phospho-peptide binding modules that typically interact with dedicated sites on their substrates through a single high affinity interaction (Pawson and Nash, 2000; Yaffe and Elia, 2001).

The mechanism that engenders a cooperative binding effect remains to be determined. In principle, multiple interactions sites might increase binding either by engaging more than one binding site on Cdc4, or by decreasing the probability of dissociation from Cdc4 (Deshaies and Ferrell, 2001; Harper, 2002; Nash et al., 2001). Cooperative interactions for the dual SH2 domain phosphatase SH-PTP2 and 14-3-3 ζ rely on two substrate binding sites for high affinity recognition of bivalent ligands (Eck et al., 1996; Yaffe et al., 1997). Notably though, inspection of the WD40 surface does not reveal any other potential ligand binding pockets or grooves that might accommodate a phosphorylated peptide motif. Although secondary weak phospho-dependent interactions might occur, it is not obvious from the structure where such putative secondary sites might be located. In favor of the probabilistic cooperativity effect, mathematical modeling suggests that cooperative behaviour arises for the interaction between a single binding site and a polyvalent ligand as a function of the number of ligand sites. In effect multiple ligand sites increase the local concentration of ligand beyond a diffusion limited threshold for escape from the receptor. In the absence of candidate secondary sites, the simplest model is favored in which Cdc4 contains only a single phospho-dependent binding site.

Comparison to other phospho-peptide binding domains. The structure of the Cdc4 WD40 domain provides direct evidence that WD40-type repeats can assemble into propellers with more than seven blades (Fulop and Jones, 1999). One consequence of the additional blade is an enlarged channel through the center of the propeller, which creates a wide binding pocket that accommodates the core Leu-pThr-Pro ligand. This pocket contrasts to all other phospho-Ser/Thr binding domains, which engage their ligand through more shallow surface contacts within loops that extend from the core domain. WD40 domains are known to interact with other proteins in at least two different modes. In the Gb transducin and TUP1 WD40 domains, the protein interaction region occurs across the top of the propeller, much as in the case of Cdc4 (Sprague et al., 2000; Wall et al., 1995). In a second mode, defined for the WD40 domain of clathrin and the b-arrestin peptide, a “peptide-in-groove” interaction occurs on the bottom edge of the propeller

between the b-strands of the second blade (ter Haar et al., 2000). Modeling of b-TrCP, which binds the consensus motif DpSGXXpS [SEQ ID NO.42] in IkBa, b-catenin, and Vpu (Yaffe and Elia, 2001), suggests that an extensive basic region on the top of the propeller will engage substrate peptides in an analogous manner to Cdc4 .

Spatial orientation of SCF substrates. A conserved feature between all E3 structures solved to date is the large distance between the substrate binding site and the catalytic site (Huang et al., 1999; Zheng et al., 2002; Zheng et al., 2000). Modeling of the Skp1-Cdc4 complex onto a model of the Skp1-Cul1-Rbx1-E2 complex suggests that the substrate is positioned for direct frontal attack by the E2 catalytic site but that a gap of some about 65Å must be bridged between the two sites, presumably by the substrate polypeptide. Unexpectedly, superposition of the WD40 domain of Cdc4 with the LRR of Skp2 does not align the defined phosphopeptide binding pocket of Cdc4 with a potential phospho-recognition site of on the concave face of the LRR repeats (Zheng et al., 2002), at least as defined by mutational analysis of the related F-box protein Grr1 in yeast (Hsiung et al., 2001). If the relative position of substrates in the WD40 versus LRR class of F-box proteins differs, spatial plasticity in substrate presentation must be possible. This notion is consistent with the fact that the HIV protein Vpu is able to redirect the specificity of the F-box protein b-TrCP by bridging bTrCP to the host cell protein CD4, in a manner that depends on phospho-dependent recognition of Vpu by b-TrCP (Margottin et al., 1998). Similarly, it is possible to create synthetic adapters that bridge the substrate recognition site of an F-box protein to an ectopic substrate (Sakamoto et al., 2001). Finally, by definition all E3s must be able to accommodate the substrate and the elongating ubiquitin chain generated by repeated catalytic cycles (Pickart, 2001). All of these points argue for considerable spatial leeway, and possibly flexibility of F-box protein orientations within the SCF catalytic cavity.

Based on the extensive Skp1-Skp2 interface, and on the inactivation of Cul1 by insertion of a flexible linker, it has been proposed that SCF complexes, and perhaps E3 enzymes in general, must present substrates to the catalytic site in a rigidly defined fashion (Zheng et al., 2002). However, the WD40 domain and the F-box of Cdc4 are linked only by a single α -helical stalk, with additional surface contact between the domains, all of which is mediated by non-conserved residues. It is thus somewhat difficult to reconcile the properties of the two F-box protein structures solved to date. Although it may be that regions truncated from Cdc4 to enable crystallization may normally help stabilize the interface, none of these regions are highly conserved between closely related Cdc4 family members. Perturbation of the rotational and translational position of the WD40 domain by introduction of additional residues into the stalk abrogates function in all cases, except for a long insertion of 12 residues. The fact that this gross structural change can be tolerated implies a degree of conformational plasticity with the catalytic cradle. This plasticity may facilitate the access of multiple ubiquitination sites within Sic1 to the catalytic center, as directed by the multiple low affinity CPD motifs in Sic1.

Insights into substrate recognition by human Cdc4. In metazoans, Cdc4 targets multiple critical regulators of cell division and development. Among these, cyclin E is a crucial substrate because its abundance must be strictly controlled in order to avoid precocious S phase entry and attendant genome instability (Spruck et al., 1999). Notably, it has been recently reported that mutational inactivation of hCDC4 occurs in several cancer cell lines that exhibit high

levels of cyclin E (Moberg et al., 2001; Strohmaier et al., 2001). In addition, hCDC4 may be mutated in up to 30% of endometrial cancers (Spruck et al., 2002). Quite strikingly, known cancer associated mutations in hCDC4 alter phosphoThr-binding residues. Given the probable requirement for homodimerization in active SCF complexes (Kominami et al., 1998; Suzuki et al., 2000), such mutations might be expected to act in a partial dominant negative manner. Other critical substrates that appear to bind Cdc4 in a phosphorylation dependent manner include SEL-10, a negative regulator of the LIN-12/Notch pathway (Hubbard et al., 1997) that targets the transcriptionally active Notch intracellular domain for degradation (Gupta-Rossi et al., 2002; Wu et al., 2001) and the presenilins, dominant mutations in which predispose to familial early onset Alzheimer's disease (Selkoe, 2001; Wu et al., 1998). Mutations that interfere with hCdc4 activity may therefore compound multiple disease phenotypes.

Yeast and human Cdc4 exhibit a high degree of structural similarity, especially in the critical substrate binding region, and moreover, Cdc4 family members are functionally conserved since the hCdc4 substrate cyclin E is efficiently degraded in yeast in a CDC4-dependent manner (Koepp et al., 2001; Nash et al., 2001; Strohmaier et al., 2001). The structure of yeast Cdc4 thus affords insights for rational drug design. Significantly, the low affinity of individual natural CDP sites that engender the requirement for multisite phosphorylation means that even compounds of moderate affinity can readily out-compete the binding of fully phosphorylated substrates (Nash et al., 2001). Naively, inhibition of hCdc4-substrate interactions would be expected to exacerbate the deregulated proliferation caused by stabilization of cyclinE, Notch-IC or presenilin. However, if Cdc4 or Cdc4-like activities limiting for growth, Cdc4 antagonists may have heightened toxicity in cells that are hypomorphic for Cdc4 function. Alternatively, disruption of hCdc4 function may cause synthetic lethal effects in combination with otherwise non-lethal mutations in functionally overlapping pathways (Tong et al., 2001).

EXAMPLE 2

The following methods were used in the investigation described in the example:

Protein expression and purification. The Cdc4 fragment employed for crystallization was deleted for residues 1-262, 602-605, 609-624, and 745-779 to remove loop regions based on sequence alignments and limited proteolysis of the intact SCF^{Cdc4} complex. Skp1 was deleted for a non-conserved loop insertion spanning residues 37-64. A GST-Skp1^{-His6}-Cdc4 complex was co-expressed from plasmid pMT3169 in B934 (DE3) bacterial strain (Stratagene) cells grown in minimal media supplemented with a mixture of selenomethionine (40 µg/ml) and methionine (0.4 µg/ml) and purified by double affinity tag chromatography (Nash et al., 2001). All mutations were constructed by standard methods using oligonucleotides listed in Table 7 and sequence verified in their entirety. Mutants were sub-cloned into pMT3055 or pMT3217 for expression in bacteria or yeast, respectively, as listed in Table 8. The WD40 domain of the helix α6 linker mutants Ala1, Ala2, Ala12, and helix α6 breaker could not be stably expressed in bacteria; the Ala12 mutant also could not be expressed in yeast.

Crystallization, data collection, structure determination and modeling. Hanging drops containing 1 µl of 20 mg/ml protein and 1.2 molar equivalents of the cyclin E derived CPD peptide (acetyl-Gly-Leu-Leu-pThr-Pro-Pro-Gln-Ser-Gly-amide) [SEQ ID NO 40] in buffer (10 mM HEPES pH 7.5, 250 mM NaCl, 1 mM DTT) were mixed with

equal volume of reservoir buffer (0.1 M Tris pH 8.5, 1.5 M ammonium sulphate). Crystals of the space group $P3_2$, ($a = 107.7\text{\AA}$, $b = 107.7\text{\AA}$, $c = 168.3\text{\AA}$, $\alpha = \gamma = 90^\circ$, $\beta = 120^\circ$), with two Cdc4–Skp1–CPD complexes in the asymmetric unit were obtained at 20°C. A Multiple Anomalous Dispersion (MAD) experiment was performed on a frozen crystal at the Advanced Photon Source (Argonne, IL) beamline BM 14-C and BM 14-D ($\lambda_1 = 0.9798\text{\AA}$, $\lambda_2 = 0.9800\text{\AA}$, $\lambda_3 = 0.9000\text{\AA}$) using a Quantum 4 ADSC CCD detector. Data processing and reduction were carried out with the HKL program suite (Otwinowski and Minor, 1997). The programs SHARP (de La Fortelle and Bricogne, 1997) and SnB (Miller et al., 1994) were used in combination to locate and refine 19 of the total 22 selenium sites. Following phasing and density modification, a model was built using O (Jones et al., 1991) and refined to 2.7 Å resolution with NCS restraints using CNS (Brunger et al., 1998) to a working R_{value} of 23.8% and R_{free} of 27.3%. Pertinent statistics for data collection and refinement are shown in Table 2. Amino acids 37-74, and 104-115 of Skp1 and amino acids 497-507 of Cdc4 were disordered and could not be modeled. 89.1% of the residues occupy the most favored regions of the Ramachandran plot, 10.8% the additional allowed region and 0.2% the generously allowed region.

Ribbons representations were generated using Ribbons (Carson, 1991), surface representations were generated using Grasp (Nicholls et al., 1991) and electron density maps were generated using O (Jones et al., 1991). A model of the ubiquitin–E2–SCF^{Cdc4}–CPD complex was generated by superposition of the Skp1 subunits of the Skp1–Cdc4–CPD structure and the Skp1–Cul1–Rbx1 structure (PDB ID 1LDK) (Zheng et al., 2002), the RING finger domains from Rbx1 in the same Skp1–Cul1–Rbx1 complex and from the Cbl subunit of the Cbl–UbcH7 structure (PDB ID 1FBV) (Zheng et al., 2000), and the E2 subunits of the Cbl–UbcH7 structure and an NMR-based Ubc1–ubiquitin model (PDB ID 1FXT) (Hamilton et al., 2001). The Skp1, RING domain and E2 subunits overlapped with RMSD values of 1.01 Å, 2.09 Å, and 2.04 Å respectively.

Cdc4 functional assays. *CDC4* mutant alleles were assessed for complementation of a *cdc4Δ* strain in a plasmid shuffle assay (Nash et al., 2001). Sensitivity to *SIC1* dosage was determined by transformation with pMT837 (*GALI-SIC1*) or pMT767 (*GALI-SIC1^{T33V}*) and plating on glucose medium or galactose medium. For in vitro capture of phospho-Sic1 by Cdc4, 0.5 μg of bacterially-expressed ^{HIS6}Sic1 was phosphorylated with immobilized Cln2–Cdc28 kinase from baculovirus-infected Sf9 cells and then incubated with 1 μg of immobilized wild type or mutant Cdc4²⁶³⁻⁷⁴⁴–GST–Skp1, at 4°C for 1hr, washed 4 times and visualized by anti-Sic1 immunoblot. For isoelectric focusing (IEF)–2D gel analyses, an evenly distributed pool of phospho-Sic1 isoforms was generated by combining different time points in a Sic1 phosphorylation reaction. 2.5 μg of the phospho-Sic1 pool was bound to 5 μg of immobilized wild type or mutant Cdc4¹⁻⁷⁴⁴–GST–Skp1. Captured isoforms were separated by denaturing IEF–2D gel electrophoresis using pH3-10NL Immobiline gel strips (Amersham) and visualized by anti-Sic1 immunoblot. Alternatively, the pool of phospho-Sic1 isoforms was incubated in solution with a ubiquitination reaction mix containing ATP, ubiquitin, yeast E1, Cdc34 and either wild type or mutant SCF^{Cdc4} complex, composed of a 1:1 ratio of bacterial Cdc4–GST–Skp1 and insect cell-produced Cdc53–Rbx1, at 30°C for 1h as previously described (Nash et al., 2001).

Results

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the outermost $\beta 9^1$ strand to run parallel to the $\beta 9$ strand. This five strand composition is unique to the fungal Cdc4 orthologs. In terms of overall structural dimensions, the WD40 domain resembles a conical frustum of 40Å diameter top surface and 50Å bottom surface, an overall thickness of 30Å and a central pore of 6Å diameter. The CPD binding site resides on the top surface of the frustum and runs across the edge of the pore, while the bottom surface of the frustum links to the F-box domain.

The F-box to WD40 domain linker. The F-box domain of Cdc4 is followed by a helical extension that forms a structured bridge to the WD40 domain. The bridge consists of two α -helices, $\alpha 5$ and $\alpha 6$, that together with helices $\alpha 3$ and $\alpha 4$ of the F-box domain form a platform and stalk-like structure that positions the WD40 domain well away from the F-box domain (Figure 2A,C). The relative orientation of the F-box domain and WD40 domain is imposed almost entirely through the integrity of the stalk-like helix $\alpha 6$, which is 30Å in length. The N-terminal end of helix $\alpha 6$ is anchored into the hydrophobic core of the F-box domain through interactions involving $\alpha 6$ residues Phe 355 and Leu 356 and F-box residues Ile 295, and Ile 296, Leu 315, Trp 316, and Leu 319 (Figure 2C). Helix $\alpha 5$ packs along side the base of helix $\alpha 6$ opposite to the F-box domain through hydrophobic interactions involving Tyr342, Leu 338 and Leu 334. The C-terminal end of helix $\alpha 6$ inserts obliquely between propeller blades $\alpha 7$ and $\alpha 8$ of the WD40 domain through van der Waals and hydrophobic interactions involving residues Trp 365 and Ile 361 with WD40 domain residues Val 687, Ile 696, Leu 726 and Phe 743 in β -propeller blades 7 and 8. Asn 364 of helix $\alpha 6$ also forms a tight hydrogen bond with the backbone carbonyl group of Phe 743 in propeller blade 8. The conservation of many of these residues, with the possible exception of those within helix $\alpha 5$, suggests that a structured linkage between the WD40 and F-box domains may be a common feature of the WD40 family F-box proteins.

The interdomain connection between the F-box and the WD40 domains of Cdc4 appears less rigidly structured than the corresponding region in hSkp2 (Figure 6A). Outside of the stalk helix $\alpha 6$, only two close contacts ($< 3.5\text{\AA}$) are observed between the WD40 domain and other regions of Cdc4 (Figure 2C). These contacts consist of hydrogen bonds between Asn684 and Arg700 in two loop regions of propeller blade 7 with Glu 323 in the $\alpha 4$ – $\alpha 5$ linker of the helical extension. Both hydrogen bonds are maintained in the two Cdc4 molecules of the crystal asymmetric unit but all three residues are poorly conserved amongst Cdc4 orthologues (Figure 1B). The lack of additional stabilizing interactions suggests that the F-box to WD40 domain linker is not exceedingly rigid, and indeed, the WD40 domain in the two Cdc4 molecules of the crystal asymmetric unit differ relative to their F-box domains by a 5° rotation about the long axis of helix $\alpha 6$. In contrast, in hSkp2 the F-box domain helix $\alpha 4$ terminates abruptly in an immediate transition to the LRR domain fold such that the adjoined domains form a rigid hydrophobic core (Schulman et al., 2000). Although the Skp2 and Cdc4 families of F-box proteins employ structurally divergent F-box interfaces, the general position of the WD40 and LLR domains are nonetheless similar (Figure 6A).

Model of the SCF^{Cdc4} E2 complex. The structure of the Skp1-Cdc4-CPD complex sheds light on how substrates are presented by the F-box protein to the E2 for ubiquitin transfer. A complete model of the E2–SCF^{Cdc4}–substrate complex consisting of ubiquitin, hUbc7, hCul1, hRbx1, ScCdc4, ScSkp1, and the CPD peptide is shown in Figure 6B.

This model is based on the reconstructed E2-SCF^{Skp2} complex derived by Pavletich and colleagues (Zheng et al., 2002), in conjunction with an NMR-based ubiquitin-E2 thioester model (Hamilton et al., 2001). Two interesting features are apparent. First, the distance between the E2 active site cysteine and the phosphate group of the bound CPD peptide is approximately 59 Å, which is similar to the spacing reported between the substrate interaction site and the E3 catalytic site in the hUbc7-Cbl structure (Zheng et al., 2000). Secondly, the WD40 domain presents the CPD peptide in a direct line-of-sight to the E2. Although the ligand-binding site on hSkp2 has not been determined, mutagenesis studies on the LRR-containing F-box protein Grr1 in yeast suggest that substrates bind to the inner side of the curved repeat surface (Hsiung et al., 2001). If the position of this site is maintained in hSkp2, then the LRR domain of Skp2 is predicted to project substrates in an orthogonal direction to that of the Cdc4 WD40 domain (Figure 6A).

Phosphopeptide recognition. The CPD binding surface represents the most conserved part of the WD40 repeat domain structure (Figure 7A-D). The central CPD sequence Leu-pThr-Pro-Pro [SEQ ID NO. 41] was modeled unambiguously in unbiased experimental electron density maps in both Skp1-Cdc4-CPD complexes of the crystal asymmetric unit (Figure 3). Interpretable electron density is also apparent for the P-2 Leu, P+3 Gln, P+4 Ser, and P+5 Gly positions, but only in one complex of the crystal asymmetric unit. The CPD peptide binds in an extended manner across β -propeller blade 2 with the N-terminus oriented towards the central pore of the WD40 domain and the C-terminus oriented towards the outer rim. Identical substrate peptide orientations and contacts were observed for an independent Skp1-Cdc4-CPD structure with a phosphopeptide derived from the transcription factor Gcn4, which is a physiological substrate of Cdc4 in yeast (Meimoun et al., 2000; Chi et al., 2001). However, of the Gcn4 peptide sequence, Phe-Leu-Pro-pThr-Pro-Val-Leu-Glu-Asp [SEQ ID NO. 43], only the core residues Pro-pThr-Pro had discernable electron density.

The CPD sequence requirements for the CPD-Cdc4 interaction are fully accounted for by structural elements in the WD40 domain. An absolute requirement for phosphorylation at Ser or Thr at the P-0 position of the CPD derives from a network of electrostatic interactions and hydrogen bonds that coordinate the P0 pThr phosphate group (Figure 7C, D). This interaction is mediated by residues that are conserved across all Cdc4 orthologs (Figure 1B). The P0 phosphate group forms direct electrostatic interactions with the guanidinium groups of Arg485, Arg467, and Arg534 and a direct hydrogen bond with the side chain of Tyr548. The side chain of Tyr548 is coordinated by stacking interactions with the guanidinium group of Arg572, which in turn is coordinated by a hydrogen bond to the side chain of Tyr574. Although Cdc4 shows a 6-fold preference for pThr over pSer (Nash et al., 2001), the structural basis for this selectivity is not obvious since the C γ methyl group of Thr is directed towards solvent and does not make contact with the WD40 domain surface.

A second absolute requirement for CPD-Cdc4 interaction rests on the P+1 proline, the side chain of which projects into a three-sided pocket on the WD40 surface. One side of this pocket is formed by the side chain of Trp 426, which packs in a coplanar manner with the P+1 proline side chain. The opposite side of this binding pocket is formed by the side chain of Arg 485 via coordination of the proline side chain and backbone carbonyl group through

van der Waals and hydrogen bonding interactions, respectively. The side chains of Thr 441 and Thr 465 define the remaining side of the P+1 proline binding pocket, with γ side chain groups composing a hydrophobic surface. The hydroxyl groups of Thr 441 and 465 orient away from the P+1 binding pocket, where they are well placed to influence binding specificity for CPD residues C-terminal to the P+1 position. Unlike Trp 426 and Arg 485, which are invariant amongst the Cdc4 orthologs, Thr 441 and Thr 465 are both substituted with Ile in the *S. pombe* Cdc4 ortholog Pop1 (Figure 1B). This substitution might restrict CPD sequences able to bind Pop1 through steric or hydrophobic constraints on residues C-terminal to the P+1 proline position.

Cdc4 displays a strong preference for the hydrophobic residues Leu/Ile/Pro at the P-1 and Leu/Ile at the P-2 CPD positions. In the crystal structure, the P-1 Leucine side-chain fits into a hydrophobic pocket composed of invariant residues Trp 426, Trp 717, and Thr 386, and the conserved hydrophobic residue Val 384. While less precisely modeled, the main chain position of Leu -2 lies in close proximity to a third hydrophobic pocket composed of the invariant residue Tyr574, and the conserved hydrophobic residues Met 590 and Leu634. The hydrophobic character of the P-1 and P-2 pockets is manifest as selection against both charged and small polar residues at these positions in the CPD consensus (Nash et al., 2001).

The WD40 phospho-recognition domain of Cdc4 is unusual in that it exhibits strong selectivity against either Arg or Lys residues in the P+2 to P+5 CPD positions, but otherwise shows no sequence preference at these positions (Nash et al., 2001). In the crystal structure, the side chain of P+2 Pro is directed towards solvent, while the main chain conformation of Pro+1 and Pro+2 causes the CPD to kink away from the peptide-binding surface from the Pro+2 position onward. As a result, only one additional contact with Cdc4 is made by the CPD following the Pro +1 position, namely a weak hydrogen bond with sub-optimal geometry between the P+4 Gln side chain and the side chain of Arg 485. Because the P+1 Pro main chain is forced away from the WD40 domain surface, the selection against basic residues in the P+2, +3, +4 and +5 positions in the CPD consensus is almost certainly due to through-space electrostatic repulsion. This effect arises from a dominant positive electrostatic potential generated by both the invariant triad of Arg residues that comprise the core pThr-Pro binding pocket, and by a radial extension of the surface due to Arg 572, Arg 443 and Lys 402, the former two of which are conserved amongst Cdc4 orthologs (Figure 7B).

A number of natural mutations detected in metazoan orthologs of Cdc4 corroborate the structure-based analysis. Two ovarian cancer cell lines bear missense mutations at conserved Arg residues that correspond to Arg 467 and Arg 534 in yeast Cdc4 (Moberg et al., 2001). In the crystal structure, these residues make direct contact with the P0 phosphate group and are essential for function (Figure 7 C, D). In a recent study of human primary endometrial tumors, mutations in phosphate-binding Arg residues equivalent to Arg 467 and Arg 485 were detected in 2 of 13 tumor samples (Spruck et al., 2002). Other cancer-associated nonsense and frameshift mutations truncate hCdc4 within the WD40 domain (Moberg et al., 2001; Strohmaier et al., 2001; Spruck et al., 2002). Similarly, all three characterized mutations in the *Drosophila ago* gene that lead to excess cell proliferation affect the WD40 domain (Moberg et al., 2001). One of these mutations, Ala1118Val, corresponding to position Ser532 in ScCdc4 substitutes a conserved small residue with a bulkier residue at the center of the critical Arg 434-Arg467-Arg534 triad (Figure 7C).

Mutational analysis of the F-box to WD40 domain linker. To probe the importance of orientation and rigidity in the F-box WD40 inter-domain linker, point mutations, insertions or deletions were introduced into the platform and stalk structure of Cdc4. None of these deletions affected the ability of the recombinant proteins to bind phospho-Sic1 *in vitro* or protein abundance *in vivo* (Figure 8A and data not shown). Introduction of the helix destabilizing residues glycine and proline into helix $\alpha 5$ did not compromise Cdc4 function *in vivo* (Figure 8B), consistent with the poorly conserved nature of this region (Figure 1B). However, two different deletions of helix $\alpha 5$ eliminated Cdc4 function *in vivo*, indicating that the F-box–WD40 domain interface is an essential structural component. Similarly, placement of helix destabilizing residues at the center of helix $\alpha 6$ or the lengthening of this helix by the insertion of one, two, three, four, 8 or 12 amino acid residues disrupted Cdc4 function *in vivo*. Helix $\alpha 6$ is thus critical for productive orientation of the WD40 domain.

Mutational analysis of the CPD binding surface. Previous mutational analysis based on sequence conservation in the Cdc4 family identified Arg467, Arg485 and Arg534 as essential for substrate binding and function in yeast (Nash et al., 2001). Two of the three corresponding residues in hCdc4, Arg 417 and Arg 457, are essential for the binding of phospho-cyclin E, while the third corresponding to Arg485 was not tested (Koepp et al., 2001). To systematically probe the role of residues that form the highly conserved peptide binding surface, a panel of Cdc4 mutants was generated and each were tested for pSic1 binding *in vitro*, complementation of a *cdc4Δ* strain and sensitivity to increased *SIC1* dosage. Four mutants, Arg467Ala, Arg485Ala, Arg534Ala, and Trp426Ala were unable to bind phospho-Sic1 *in vitro* or complement a *cdc4Δ* strain, but were fully competent for Skp1 binding (Figure 8A, B). The essential function of these residues is not confined to elimination of Sic1 because none of the corresponding mutant alleles were able to rescue a *cdc4Δ sic1Δ* strain. These results reflect the critical structural role played by these residues in coordination of the P0 phosphate and the P+1 proline of the CPD. Mutation of the remaining phosphate-coordinating residue, Tyr548, did not cause loss of viability but did result in dosage sensitivity to *SIC1^{Thr33Val}*, which encodes a partially stabilized version of Sic1 (Figure 8C). Mutation of Arg 572 had the same effect, as befits the observed stacking interaction between this residue and Tyr 548. Although both mutants were severely impaired for binding to phospho-Sic1 *in vitro*, this effect may be exacerbated by the tendency of these recombinant proteins to aggregate. In summary, the six residues that directly or indirectly coordinate the primary pThr-Pro core motif are critical for CPD recognition *in vitro* and Cdc4 function *in vivo*.

Disruption of residues that confer selection at the P-2, P-1 and P+2 to P+5 positions had only modest effects on the ability of Cdc4 to target pSic1. A Trp717Asn mutation predicted to disrupt the P-1 pocket conferred sensitivity to dosage of *SIC1^{Thr33Val}*, but did not overtly affect the pSic1-Cdc4 interaction *in vitro*. Individual mutations in all other residues that are well positioned to affect substrate selection, namely Arg443Ala, Arg443Asp, Lys402Ala, Tyr574Phe and Val384Asn were indistinguishable from wild type in each of the assays used. Substrate selection residues on the WD40 surface thus contribute only modestly if at all to the essential function of Cdc4. As described below, however, these residues play a subtle but critical role in setting the phosphorylation threshold for the CPD-Cdc4 interaction.

Modulation of CPD substrate selectivity. A critical feature of the Sic1-Cdc4 interaction is the requirement for phosphorylation of Sic1 on multiple sites. To enforce this requirement, each of the phosphorylation sites in the native Sic1 sequence are sub-optimal in one or more respects (Figure 9A). The Cdc4-CPD structure suggests that selectivity against basic residues may be due to electrostatic repulsion generated from the conserved patch of basic residues in and around the CPD binding pocket, while selection for hydrophobic residues arises from the P-1 pocket that is composed in part by Val 384 and Trp717. To examine the basis for selection against sub-optimal CPD motifs, the effects of mutations in non-essential residues in these two regions on the multisite phosphorylation requirement for Sic1 recognition were assessed.

The ability of Cdc4 to capture various phosphoisoforms of wild type Sic1 from a pool of recombinant Sic1 that had been phosphorylated to various extents by Cln2-Cdc28 was monitored. As resolved by isoelectric focusing, this pool contained roughly equal amounts of Sic1 phosphorylated on 1, 2, 3, 4, 5, 6, 7, 8 and 9 sites. Wild type Cdc4 was only able to capture Sic1 phosphorylated on six or more sites (Figure 9B). This result formally demonstrates the transition in binding affinity between 5 and 6 phosphorylation sites, as initially inferred from capture of a series of Sic1 phosphorylation site mutants by Cdc4 (Nash et al., 2001). The role of positive electrostatic potential in selecting against sub-optimal CPD sequences with basic residues at C-terminal positions was tested with the Lys402Ala Arg443Asp double mutant. This mutant was able to select Sic1 phosphoisoforms that contained as few as three phosphorylation sites (Figure 9B). The ability of the Lys402Ala Arg443Asp double mutant to capture lower phosphorylated forms of Sic1 is also evident in one-dimensional SDS-PAGE (Figure 8A). Similarly, perturbation of the P-1 hydrophobic pocket with a Val384Asn Trp717Asn double mutation allowed capture of Sic1 phosphorylated on as few as four sites. These in vitro binding results were recapitulated in solution-based in vitro ubiquitination assays with wild type and mutant forms of Cdc4. Both double mutant forms of Cdc4 were able to convert Sic1 phosphorylated on four or five sites to oligo-ubiquitinated species, whereas wild type Cdc4 was unable to do so (Figure 9C). The double mutants were, however, less efficient than wild type at elaborating fully ubiquitinated species of phospho-Sic1, perhaps because of protein stability effects or interference with catalytic steps after substrate binding. This interpretation is consistent with the sensitivity of strains bearing the double mutant alleles to *SIC1^{Thr33Val}* dosage (Figure 8B). Overall, re-engineering of negative selection residues in the Cdc4 WD40 domain supports the notion that the series of sub-optimal CPD motifs in Sic1 sets a high phosphorylation threshold for its recognition by Cdc4.

Discussion

The structure of the Skp1-Cdc4-CPD complex provides direct visualization of substrate orientation within an SCF complex. Insights gained from the structure include the unexpectedly frail interface between the F-box and the WD40 repeat domain, the basis for dedicated pThr-Pro dipeptide recognition by a novel eight-blade WD40 propeller, and a detailed understanding of the basis for selection against natural CPD sequences. The latter feature appears to be tailored to enforce multisite phosphorylation dependent degradation of Sic1, which in turn would help engender a highly cooperative onset of DNA replication (Nash et al., 2001). Similar principles may well operate for other Cdc4 substrates, including cyclin E, Notch^{IC} and presenilin in mammalian cells (Strohmaier et al., 2001; Lai, 2002; Selkoe,

2001). Because yeast and human Cdc4 are structurally and functionally analogous (Nash et al., 2001; Strohmaier et al., 2001; Koepp et al., 2001), the structure of yeast Cdc4 affords obvious insights for pharmacological modulation of hCdc4 function in these pathways. Interestingly, a significant proportion of characterized human and fly *CDC4* mutations alter residues in the CPD binding pocket. Given the probable requirement for homodimerization in active SCF complexes (Wolf et al., 1999), such mutations might act in a partial dominant negative manner to confer a growth advantage in the heterozygous state.

Phospho-recognition by Cdc4. The specificity of phosphorylation-dependent recognition by the WD40 domain of Cdc4 is governed by three main determinants: (i) a dedicated pThr-Pro binding pocket; (ii) a deep hydrophobic pocket that selects hydrophobic residues N-terminal to the phosphorylation site, and (iii) a through space electrostatic selection against basic residues C-terminal to the phosphorylation site. As for all documented phospho-dependent lipid/protein recognition modules, the Cdc4 WD40 domain employs arginine residues to directly contact the phosphate group of the ligand. However, unlike most domains in which adjacent residues impose subtle effects on specificity (Yaffe and Elia, 2001), the P+1 proline is an integral component of the core binding determinant (Nash et al., 2001). In the Cdc4-CPD co-crystal, ligand residues are locked in place by direct contact of the phosphate and proline carbonyl groups with three conserved and essential Arg residues, while the proline side chain inserts into a tight hydrophobic pocket formed by Trp426, Thr441, and Thr465. Because the phospho-binding pocket infrastructure has no obvious demarcation between the pThr and Pro binding sites, the Cdc4 WD40 domain is in effect a dedicated pThr-Pro binding module.

Comparison to other peptide recognition modules. Interesting parallels can be drawn between the Cdc4 WD40 domain, 14-3-3 domains and the class IV WW domains, which all have the ability to recognize phospho-Ser/Thr epitopes in the context of adjacent proline residues (Yaffe and Elia, 2001). The interaction of the Pin1 class IV WW domain with a pSer-Pro peptide differs from Cdc4 in that it does not rely on an extensive network of Arg residues for phosphate coordination (Verdecia et al., 2000). However, a striking similarity between Pin1 and Cdc4 lies in the P+1 proline binding pocket, which in both cases depend on a highly conserved tryptophan side chain to engage the P+1 proline pyrrolidine ring through a coplanar interaction. In contrast to Cdc4, Pin1 actually displays a preference for Arg in the P+2 position, such that the binding specificity of the pSer-Pro recognition domain closely matches that of the targeting CDK enzymes.

14-3-3 domains bind pSer epitopes with a preference, but not an absolute requirement, for proline residues at the P+2 position (Yaffe et al., 1997). This less stringent selection arises because the 14-3-3 proline binding pocket is able to accommodate other residues with propensity to form β -turns. Interestingly, the proline preferences in both the 14-3-3 and Cdc4 WD40 domains give rise to the same qualitative effect: in each case the prolines terminate direct interactions between the peptide and the ligand binding domain by orienting the peptide away from the domain surface. In the case of Cdc4, biologically significant electrostatic effects operate in spite of the loss of direct peptide contact. Physiologically relevant substrate anti-selection mediated by charge repulsion is unique amongst known protein interaction modules.

The structure of the Cdc4 WD40 domain provides direct evidence that WD40-type repeats can assemble into propellers with more than seven blades (Fulop and Jones, 1999). WD40 domains are known to interact with other proteins in at least two different modes, either across the front face of the propeller, as in the case of Cdc4, or on the outer edge of the propeller as in the case of clathrin (ter Haar et al., 2000). Modeling of the F-box protein β -TrCP, which binds the doubly phosphorylated consensus motif DpSGXXpS [SEQ ID NO. 42] in I κ B α , β -catenin, and Vpu (Yaffe and Elia, 2001), reveals an extensive conserved basic region on the front face of the propeller, which may engage substrate phosphopeptides in an analogous manner to Cdc4.

Spatial orientation of SCF substrates. A conserved feature between all E3 structures solved to date is the substantial distance between the substrate binding site and the catalytic site (Huang et al., 1999; Zheng et al., 2000; Zheng et al., 2002). Superposition of the Skp1-Cdc4 complex onto a model of the Skp1-Cul1-Rbx1-E2-ubiquitin complex suggests that the substrate is positioned for direct frontal attack by the E2 catalytic site, but that a gap of some 59Å between the two sites must be bridged, presumably by the substrate polypeptide. The disordered structure of Sic1 lends itself to this possibility (Nash et al., 2001). Intriguingly, overlay of the WD40 domain of Cdc4 with the LRR of Skp2 does not align the defined phosphopeptide binding pocket of Cdc4 with a potential phospho-recognition site on the concave face of the LRR repeats (Zheng et al., 2002), at least as defined by mutational analysis of the related F-box protein Grr1 in yeast (Hsiung et al., 2001). If the relative position of substrates in the WD40 versus LRR class of F-box proteins do in fact differ, spatial leeway in substrate presentation must be possible.

Based on the extensive Skp1-Skp2 interface, and on the inactivation of Cul1 by insertion of a flexible linker, it has been proposed that SCF complexes, and perhaps E3 enzymes in general, must present substrates to the catalytic site in a rigidly defined fashion (Zheng et al., 2002). Unexpectedly, the WD40 domain and the F-box of Cdc4 are linked only by a single α -helical stalk, with very limited additional contacts. Despite the lack of sequence conservation in the α helix 6 structure that supports the WD40 domain, spatial constraints are nevertheless evident, as shown by the sensitivity of the structure to rotational and translational shifts caused by insertion of additional residues into the stalk. It is also possible that regions truncated from Cdc4 to enable crystallization may normally help stabilize the inter-domain interface.

Cooperativity in substrate selection by Cdc4. The properties of the Cdc4 phosphopeptide binding module differ from those of other known modules in the important respect that the interaction with core recognition elements is partially offset by specific selection against basic residues in the substrate peptide. This feature establishes an intrinsic antagonism between the recognition mechanism and the targeting CDK kinases, which prefer Ser/Thr-Pro sites with C-terminal basic residues (Endicott et al., 1999). Significantly, all of the natural CPD motifs in Sic1 contain one or more mismatches to the optimal CPD consensus. This system based on positive and negative ligand selection may not only set an elevated threshold for kinase activity, but may also allow the threshold to be precisely tuned for any given substrate by varying the number, spacing and properties of each site. Thus, Cdc4 is able to target numerous critical factors for phosphorylation-dependent degradation, including the Cdk inhibitor Sic1, the CDK inhibitor and polarization factor Far1, the replication initiator Cdc6 and the transcription factor Gcn4, all of which may be

controlled with different kinetics and different phosphorylation thresholds (Patton et al., 1998). In one extreme, typified by Gcn4 and cyclin E, the substrate may contain a high affinity site that is augmented by several minor low affinity sites (Meimoun et al., 2000; Chi et al., 2001; Strohmaier et al., 2001). In the other, more akin to Sic1, a large number of weak sites may cooperate to drive high affinity binding only when a phosphorylation threshold is reached.

As shown here, mutation of either the distal basic selection region or the P-1 pocket in Cdc4 shifts the binding equilibrium to lower phosphorylated forms of Sic1, which, in the absence of other structural effects that may compromise Cdc4, would be predicted to cause premature DNA replication and genome stability (Nash et al., 2001). These features distinguish Cdc4 from other known phospho-peptide binding modules characterized to date that typically interact with dedicated sites on their substrates through a single high affinity interaction.

The mechanism that underlies the cooperative binding transition of the phospho-Sic1-Cdc4 interaction between five and six phosphorylation sites remains to be determined. In principle, multiple interactions sites might increase binding by engaging more than one binding site on Cdc4 (Figure 9D). This type of cooperative interaction is common in biological systems, as in the avidity of antibodies for polyvalent ligands and pathogen-host interactions (Mammen et al., 1998). Analogous cooperative binding interactions occur in signaling pathways. For instance, the dual SH2 domain phosphatase SH-PTP2 and the 14-3-3 ζ protein both engage two substrate binding sites on their respective ligands (Eck et al., 1996; Yaffe et al., 1997). However, inspection of the Cdc4 WD40 domain surface does not reveal any obvious ligand binding sites that might accommodate a second phosphorylated peptide motif, nor is there any biochemical evidence for secondary binding sites (Nash et al., 2001). In addition, the wide range of substrates and site spacing accommodated by Cdc4, including random concatamers of synthetic CPD sites (Nash et al., 2001), is a priori difficult to explain by two or more fixed binding sites on Cdc4.

Instead, a model is favored that requires only a single phospho-dependent binding site on Cdc4 (Figure 9D). In this scheme, phosphorylation of multiple CPD sites on Sic1 increases the local concentration of sites around Cdc4 once the first CPD site is bound, to the point where diffusion limited escape from the receptor is overwhelmed by the probability of re-binding of any one CPD site. In a sense, Sic1 becomes kinetically trapped in close proximity to Cdc4. Mathematical modeling of an idealized polyvalent ligand-monovalent receptor interaction indicates that the rate of ligand escape from the receptor exhibits a negative exponential dependence on the number of ligand sites. The term *allovalent* is proposed to describe the ability of multiple weak spatially separated ligand sites to cooperatively interact with a single receptor site. The prevalence of multisite phosphorylation (Cohen, 2000), and indeed of polyvalent ligands in general (Mammen et al., 1998), suggests that this type of behavior may underlie many biological processes.

The present invention is not to be limited in scope by the specific embodiments described herein, since such embodiments are intended as but single illustrations of one aspect of the invention and any functionally equivalent embodiments are within the scope of this invention. Indeed, various modifications of the invention in addition to those shown and described herein will become apparent to those skilled in the art from the foregoing description and accompanying drawings. Such modifications are intended to fall within the scope of the appended claims. In particular

it will be appreciated that the references to specific amino acid residues for particular a SCF complexes, and components thereof (e.g. F-box protein) illustrated in the Tables and Figures, in no way limits the scope of the invention and it will be appreciated that a person skilled in the art could determine the specific corresponding amino acid residues for other SCF complexes and components thereof.

5 All publications, patents and patent applications referred to herein are incorporated by reference in their entirety to the same extent as if each individual publication, patent or patent application was specifically and individually indicated to be incorporated by reference in its entirety. All publications, patents and patent applications mentioned herein are incorporated herein by reference for the purpose of describing and disclosing the cell lines, vectors, methodologies etc. which are reported therein which might be used in connection with the invention. Nothing
10 herein is to be construed as an admission that the invention is not entitled to antedate such disclosure by virtue of prior invention.

It must be noted that as used herein and in the appended claims, the singular forms "a", "an", and "the" include plural reference unless the context clearly dictates otherwise. Thus, for example, reference to "a host cell" includes a plurality of such host cells, reference to the "antibody" is a reference to one or more antibodies and
15 equivalents thereof known to those skilled in the art, and so forth.

Table 1.
Data Collection, Structure Determination, and Refinement Statistics

		Peak	Inflection	Remote
5	Wavelength (Å)	0.9798	0.9800	0.9000
	Resolution (Å)	2.8	2.9	2.7
	R _{sym} (%)	5.9 (38.7)	6.1 (36.1)	5.0 (28.9)
	Total Reflections	311509	187010	298371
10	Unique Reflections	107167	96027	116218
	Completeness (%)	99.8 (99.1)	99.3 (98.3)	97.7 (93.6)
	I/σ	9.9 (2.7)	7.4 (2.1)	10.1 (2.9)
	Phasing Power			
15	Refinement statistics			
	Resolution range (Å)	20-2.8		
	Reflections	103863		
	R _{factor} /R _{free} (%)	24.09/28.71		
20	Rms deviations			
	Bonds (Å)	0.0091		
	Angles (°)	1.3453		
25	Space group P3 ₂ : a = b = 107.7 Å, c = 168.3 Å; a = b = 90°, c = 120° ; Two molecules per asymmetric unit.			

¹Data for the highest resolution shell (2.90-2.80 Å)

30 ²R_{sym} = 100 × Σ|I - <I>|/Σ<I>, where I is the observed intensity and <I> is the average intensity from multiple observations of symmetry-related reflections.

³Phasing power for isomorphous and anomalous acentric reflections, where phasing power = <(|F_{h,c}| / phase-integrated lack of closure)>.

⁴R_{free} was calculated with 8.8% of the data.

Table 2.
Data Collection, Structure Determination, and Refinement Statistics

<i>Phasing Statistics</i>		Peak	Inflection	Remote
5				
	Wavelength (Å)	0.9798	0.9800	0.9000
	Resolution (Å)	2.8 (2.9-2.8)	2.9 (3.0-2.9)	2.7 (2.8-2.7)
	R _{sym} (%)	5.9 (37.2)	6.1 (36.1)	5.0 (28.9)
10	Total Reflections	311509	187010	298371
	Unique Reflections	107167	96027	116218
	Completeness (%)	99.8 (99.1)	99.3 (98.3)	97.7 (93.6)
	I/σ	9.9 (2.7)	7.4 (2.1)	10.1 (2.9)
	Phasing Power (ISO/ANO)	5.2/1.3	4.0/0.94	0/0.91
15	<i>Refinement statistics (remote wavelength)</i>			
	R _{resolution} range (Å)	20-2.7	# protein atoms	9364
	Reflections	113960	# water molecules	72
20	R _{factor} /R _{free} (%)	23.8/27.3		
	R _{ms} deviations			
	Bonds (Å)	0.0089		
	Angles (°)	1.42		
25	Space group P3 ₂ ; a = b = 107.7 Å, c = 168.3 Å; a = b = 90°, c = 120° Two Skp1-Cdc4-CPD complexes per asymmetric unit			
30	<p>Numbers given in parantheses refer to data for the highest resolution shell.</p> <p>¹R_{sym} = 100 × Σ I - <I> /Σ<I>, where I is the observed intensity and <I> is the average intensity from multiple observations of symmetry-related reflections.</p> <p>²Phasing power for isomorphous and anomalous acentric reflections, = <[F_h(calc)/phase-integrated lack of closure]>.</p> <p>³R_{free} was calculated with 8.8% of the data.</p>			

Table 3.
Atomic Contacts of a Substrate Binding Pocket

No. of Atomic Interaction	CDC4 WD40 Motif Atomic Contact	CDC4 atomic Contact	CPD Motif Atomic Contact
1	Ile 295 Ile296 Leu 315 Trp 316 Leu 319	Phe 255 Leu356	
2	Val 687 Ile 696 Leu 726 Phe 743	Trp 365 Ile 364	
3	Phe 743	Asn 364	
4	Asn 684 Arg 700	Glu 323	
5	Arg 485 Arg 467 Arg 534 Tyr 548		PO pTyr Phosphate
6	Trp 426 Arg 485 Thr 386 Thr 441 Thr 465		P+1 Proline side chain
7	Trp 426 Trp 717 Thr 386 Val 384		P+1 Leucine side chain
8	Tyr 574 Thr 386 Val 384		Leucine +2

Table 4.
Atomic Contacts of a Substrate Binding Pocket

No. of Atomic Interaction	CDC4 WD40 Motif/F-box Domain Atomic Contact	CDC4 atomic Contact	CPD Motif Atomic Contact	Atomic Interaction Property
1	Ile 295 Ile296 Leu 315 Trp 316 Leu 319	Phe 355 Leu356		hydrophobic interactions and van der Wals interactions
2	Val 687 Ile 696 Leu 726 Phe 743	Trp 365 Ile 361		van der Wals and hydrophobic interactions
3	Phe 743	Asn 364		hydrogen bond
4	Asn 684 Arg 700	Glu 323		hydrogen bonds
5	Arg 485 Arg 467 Arg 534 Tyr 548		PO pTyr or pSer Phosphate at P-O position of CPD	electrostatic interactions hydrogen bond
6	Trp 426 Arg 485 Thr 441 Thr 465		P+1 Proline side chain and backbone carbonyl of CPD	hydrogen and van der Wals hydrophobic interactions
7	Trp 426 Trp 717 Thr 386 Val 384		P-1 Leucine (or Ile/Pro) side chain	hydrophobic interactions
8	Tyr 574 Met 590 Leu 634		Leucine -2 Leu/Ile at P-2 position	hydrophobic interactions
9.	Tyr 342 Leu 338 Leu 334			hydrophobic interactions

Table 5

Determinants of pThr-Pro binding

[illegible]

Table 6

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REMARK peptide link removed (applied DPEP): from A    31    to A    45
REMARK peptide link removed (applied DPEP): from A    73    to A    86
REMARK peptide link removed (applied DPEP): from B   496    to B   508
5  REMARK peptide link removed (applied DPEP): from C    31    to C    45
REMARK peptide link removed (applied DPEP): from C    73    to C    86
REMARK peptide link removed (applied DPEP): from D   496    to D   508
REMARK peptide link removed (applied DPPP): from E     4     to E     5
REMARK coordinates from minimization and B-factor refinement
10  REMARK refinement resolution: 20 - 2.8 A
REMARK starting r= 0.2415 free_r= 0.2846
REMARK final      r= 0.2409 free_r= 0.2871
REMARK rmsd bonds= 0.009114  rmsd angles=  1.34531
REMARK B rmsd for bonded mainchain atoms=  1.230  target= 1.5
15  REMARK B rmsd for bonded sidechain atoms=  1.778  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.103  target= 2.0
REMARK B rmsd for angle sidechain atoms=  2.675  target= 2.5
REMARK target= mlf  final wa= 2.77695
REMARK final rweight=  0.1078 (with wa= 2.77695)
20  REMARK md-method= torsion  annealing schedule= constant
REMARK starting temperature= 2000  total md steps= 1 * 100
REMARK cycles= 2 coordinate steps= 20 B-factor steps= 10
REMARK sg= P3(2) a= 107.669 b= 107.669 c= 168.3 alpha= 90 beta= 90 gamma= 120
REMARK topology file 1 : CNS_TOPPAR:protein.top
25  REMARK topology file 2 : CNS_TOPPAR:dna-rna.top
REMARK topology file 3 : CNS_TOPPAR:water.top
REMARK topology file 4 : CNS_TOPPAR:ion.top
REMARK topology file 5 : CNS_TOPPAR:tpo.top
REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
30  REMARK parameter file 2 : CNS_TOPPAR:dna-rna_rep.param
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : CNS_TOPPAR:tpo.param
REMARK molecular structure file: automatic
35  REMARK input coordinates: 36mod1.pdb
REMARK reflection file= remote.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 2.8
REMARK initial B-factor correction applied to fobs :
40  REMARK  B11=  1.580 B22=  1.580 B33= -3.160
REMARK  B12= -3.767 B13=  0.000 B23=  0.000
REMARK B-factor correction applied to coordinate array B:  0.915
REMARK bulk solvent: density level= 0.324998 e/A^3, B-factor= 34.4718 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
45  REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK anomalous diffraction data was input
REMARK theoretical total number of refl. in resol. range: 107240 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0): 3377 (  3.1 % )
REMARK number of reflections rejected: 0 (  0.0 % )
50  REMARK total number of reflections used: 103863 ( 96.9 % )
REMARK number of reflections in working set: 93784 ( 87.5 % )
REMARK number of reflections in test set: 10079 (  9.4 % )
CRYST1 107.669 107.669 168.300 90.00 90.00 120.00 P 32

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REMARK FILENAME="ref37.pdb"

REMARK DATE:28-Jun-2002 13:23:24

created by user: orlicky

REMARK VERSION:1.1

	ATOM	1	CB	SER	A	2	72.279	75.039	74.638	1.00	40.45	A
5	ATOM	2	OG	SER	A	2	72.875	75.230	73.368	1.00	36.62	A
	ATOM	3	C	SER	A	2	70.142	75.473	73.446	1.00	40.01	A
	ATOM	4	O	SER	A	2	69.547	74.397	73.338	1.00	39.92	A
	ATOM	5	N	SER	A	2	70.277	75.520	76.026	1.00	40.09	A
	ATOM	6	CA	SER	A	2	70.953	75.797	74.713	1.00	40.80	A
10	ATOM	7	N	ASN	A	3	70.145	76.398	72.482	1.00	38.91	A
	ATOM	8	CA	ASN	A	3	69.428	76.196	71.221	1.00	37.67	A
	ATOM	9	CB	ASN	A	3	68.480	77.367	70.926	1.00	38.01	A
	ATOM	10	CG	ASN	A	3	67.193	77.305	71.736	1.00	38.13	A
	ATOM	11	OD1	ASN	A	3	66.616	76.236	71.944	1.00	38.39	A
15	ATOM	12	ND2	ASN	A	3	66.733	78.458	72.184	1.00	36.20	A
	ATOM	13	C	ASN	A	3	70.310	75.996	69.990	1.00	35.89	A
	ATOM	14	O	ASN	A	3	71.503	76.275	69.995	1.00	34.48	A
	ATOM	15	N	VAL	A	4	69.685	75.500	68.928	1.00	36.46	A
	ATOM	16	CA	VAL	A	4	70.343	75.275	67.639	1.00	33.96	A
20	ATOM	17	CB	VAL	A	4	70.545	73.750	67.383	1.00	33.36	A
	ATOM	18	CG1	VAL	A	4	70.533	73.449	65.916	1.00	33.70	A
	ATOM	19	CG2	VAL	A	4	71.855	73.295	67.985	1.00	34.50	A
	ATOM	20	C	VAL	A	4	69.415	75.889	66.584	1.00	31.88	A
	ATOM	21	O	VAL	A	4	68.209	76.036	66.818	1.00	31.04	A
25	ATOM	22	N	VAL	A	5	69.972	76.282	65.443	1.00	31.25	A
	ATOM	23	CA	VAL	A	5	69.146	76.853	64.376	1.00	31.10	A
	ATOM	24	CB	VAL	A	5	69.458	78.346	64.086	1.00	31.85	A
	ATOM	25	CG1	VAL	A	5	68.586	78.825	62.927	1.00	32.81	A
	ATOM	26	CG2	VAL	A	5	69.188	79.192	65.314	1.00	31.47	A
30	ATOM	27	C	VAL	A	5	69.339	76.075	63.089	1.00	29.35	A
	ATOM	28	O	VAL	A	5	70.448	75.952	62.588	1.00	29.57	A
	ATOM	29	N	LEU	A	6	68.232	75.561	62.574	1.00	28.63	A
	ATOM	30	CA	LEU	A	6	68.206	74.777	61.355	1.00	28.72	A
	ATOM	31	CB	LEU	A	6	67.299	73.558	61.559	1.00	27.60	A
35	ATOM	32	CG	LEU	A	6	67.585	72.619	62.739	1.00	25.63	A
	ATOM	33	CD1	LEU	A	6	66.684	71.402	62.592	1.00	24.10	A
	ATOM	34	CD2	LEU	A	6	69.043	72.205	62.781	1.00	21.89	A
	ATOM	35	C	LEU	A	6	67.667	75.632	60.208	1.00	28.54	A
	ATOM	36	O	LEU	A	6	66.577	76.200	60.316	1.00	28.48	A
40	ATOM	37	N	VAL	A	7	68.416	75.740	59.112	1.00	27.74	A
	ATOM	38	CA	VAL	A	7	67.945	76.548	57.978	1.00	25.90	A
	ATOM	39	CB	VAL	A	7	69.092	77.413	57.366	1.00	25.69	A
	ATOM	40	CG1	VAL	A	7	68.515	78.450	56.403	1.00	25.12	A
	ATOM	41	CG2	VAL	A	7	69.889	78.077	58.450	1.00	22.70	A
45	ATOM	42	C	VAL	A	7	67.374	75.650	56.869	1.00	24.30	A
	ATOM	43	O	VAL	A	7	68.069	74.768	56.337	1.00	21.91	A
	ATOM	44	N	SER	A	8	66.111	75.881	56.522	1.00	23.21	A
	ATOM	45	CA	SER	A	8	65.453	75.091	55.486	1.00	23.15	A
	ATOM	46	CB	SER	A	8	63.966	75.433	55.375	1.00	21.22	A
50	ATOM	47	OG	SER	A	8	63.794	76.735	54.826	1.00	20.44	A
	ATOM	48	C	SER	A	8	66.093	75.428	54.167	1.00	25.17	A
	ATOM	49	O	SER	A	8	66.851	76.389	54.054	1.00	27.53	A
	ATOM	50	N	GLY	A	9	65.782	74.635	53.155	1.00	26.78	A
	ATOM	51	CA	GLY	A	9	66.329	74.914	51.847	1.00	26.99	A

	ATOM	52	C	GLY	A	9	65.726	76.208	51.320	1.00	27.95	A
	ATOM	53	O	GLY	A	9	66.120	76.682	50.256	1.00	29.65	A
	ATOM	54	N	GLU	A	10	64.762	76.782	52.039	1.00	26.66	A
	ATOM	55	CA	GLU	A	10	64.160	78.025	51.582	1.00	25.22	A
5	ATOM	56	CB	GLU	A	10	62.637	77.927	51.610	1.00	24.78	A
	ATOM	57	CG	GLU	A	10	62.045	76.721	50.905	1.00	24.26	A
	ATOM	58	CD	GLU	A	10	60.543	76.567	51.203	1.00	27.17	A
	ATOM	59	OE1	GLU	A	10	59.747	77.407	50.727	1.00	27.67	A
	ATOM	60	OE2	GLU	A	10	60.144	75.617	51.929	1.00	28.38	A
10	ATOM	61	C	GLU	A	10	64.598	79.236	52.416	1.00	25.50	A
	ATOM	62	O	GLU	A	10	63.853	80.213	52.538	1.00	24.72	A
	ATOM	63	N	GLY	A	11	65.794	79.164	52.995	1.00	25.06	A
	ATOM	64	CA	GLY	A	11	66.299	80.264	53.792	1.00	25.04	A
	ATOM	65	C	GLY	A	11	65.740	80.473	55.192	1.00	25.64	A
15	ATOM	66	O	GLY	A	11	66.399	81.110	56.016	1.00	25.60	A
	ATOM	67	N	GLU	A	12	64.552	79.946	55.483	1.00	26.56	A
	ATOM	68	CA	GLU	A	12	63.945	80.113	56.806	1.00	27.47	A
	ATOM	69	CB	GLU	A	12	62.510	79.614	56.782	1.00	26.92	A
	ATOM	70	CG	GLU	A	12	61.661	80.451	55.874	1.00	32.01	A
20	ATOM	71	CD	GLU	A	12	60.215	80.003	55.841	1.00	35.92	A
	ATOM	72	OE1	GLU	A	12	59.912	78.942	55.244	1.00	37.74	A
	ATOM	73	OE2	GLU	A	12	59.367	80.716	56.419	1.00	39.01	A
	ATOM	74	C	GLU	A	12	64.705	79.459	57.951	1.00	28.74	A
	ATOM	75	O	GLU	A	12	65.222	78.345	57.826	1.00	29.61	A
25	ATOM	76	N	ARG	A	13	64.804	80.170	59.069	1.00	29.55	A
	ATOM	77	CA	ARG	A	13	65.513	79.615	60.207	1.00	30.68	A
	ATOM	78	CB	ARG	A	13	66.457	80.651	60.832	1.00	32.30	A
	ATOM	79	CG	ARG	A	13	66.654	81.907	60.002	1.00	34.52	A
	ATOM	80	CD	ARG	A	13	67.459	82.959	60.756	1.00	35.08	A
30	ATOM	81	NE	ARG	A	13	68.816	82.514	61.051	1.00	36.91	A
	ATOM	82	CZ	ARG	A	13	69.454	82.778	62.188	1.00	37.09	A
	ATOM	83	NH1	ARG	A	13	68.846	83.485	63.129	1.00	35.87	A
	ATOM	84	NH2	ARG	A	13	70.691	82.328	62.391	1.00	37.00	A
	ATOM	85	C	ARG	A	13	64.511	79.130	61.238	1.00	29.61	A
35	ATOM	86	O	ARG	A	13	63.494	79.783	61.506	1.00	29.30	A
	ATOM	87	N	PHE	A	14	64.809	77.962	61.789	1.00	28.74	A
	ATOM	88	CA	PHE	A	14	63.980	77.337	62.797	1.00	28.90	A
	ATOM	89	CB	PHE	A	14	63.507	75.945	62.356	1.00	27.81	A
	ATOM	90	CG	PHE	A	14	62.614	75.946	61.147	1.00	26.25	A
40	ATOM	91	CD1	PHE	A	14	63.149	75.925	59.867	1.00	25.67	A
	ATOM	92	CD2	PHE	A	14	61.235	75.955	61.291	1.00	27.94	A
	ATOM	93	CE1	PHE	A	14	62.324	75.912	58.745	1.00	25.90	A
	ATOM	94	CE2	PHE	A	14	60.393	75.942	60.174	1.00	27.89	A
	ATOM	95	CZ	PHE	A	14	60.940	75.921	58.896	1.00	26.23	A
45	ATOM	96	C	PHE	A	14	64.847	77.185	64.032	1.00	30.32	A
	ATOM	97	O	PHE	A	14	66.004	76.760	63.959	1.00	30.71	A
	ATOM	98	N	THR	A	15	64.305	77.558	65.176	1.00	32.94	A
	ATOM	99	CA	THR	A	15	65.067	77.412	66.396	1.00	34.55	A
	ATOM	100	CB	THR	A	15	64.910	78.650	67.275	1.00	34.81	A
50	ATOM	101	OG1	THR	A	15	65.362	79.797	66.548	1.00	35.82	A
	ATOM	102	CG2	THR	A	15	65.737	78.509	68.541	1.00	36.02	A
	ATOM	103	C	THR	A	15	64.535	76.179	67.119	1.00	34.29	A
	ATOM	104	O	THR	A	15	63.358	75.830	66.984	1.00	35.01	A
	ATOM	105	N	VAL	A	16	65.398	75.501	67.859	1.00	34.16	A

	ATOM	106	CA	VAL	A	16	64.954	74.330	68.592	1.00	36.47	A
	ATOM	107	CB	VAL	A	16	64.597	73.166	67.628	1.00	38.19	A
	ATOM	108	CG1	VAL	A	16	65.697	72.981	66.579	1.00	37.94	A
	ATOM	109	CG2	VAL	A	16	64.403	71.884	68.421	1.00	40.71	A
5	ATOM	110	C	VAL	A	16	65.992	73.862	69.601	1.00	36.55	A
	ATOM	111	O	VAL	A	16	67.199	74.020	69.398	1.00	36.18	A
	ATOM	112	N	ASP	A	17	65.511	73.294	70.699	1.00	36.09	A
	ATOM	113	CA	ASP	A	17	66.398	72.817	71.750	1.00	36.61	A
	ATOM	114	CB	ASP	A	17	65.586	72.082	72.812	1.00	38.44	A
10	ATOM	115	CG	ASP	A	17	66.458	71.416	73.840	1.00	40.95	A
	ATOM	116	OD1	ASP	A	17	66.418	70.164	73.924	1.00	43.10	A
	ATOM	117	OD2	ASP	A	17	67.184	72.137	74.556	1.00	41.69	A
	ATOM	118	C	ASP	A	17	67.499	71.902	71.196	1.00	35.77	A
	ATOM	119	O	ASP	A	17	67.218	70.903	70.543	1.00	33.05	A
15	ATOM	120	N	LYS	A	18	68.757	72.245	71.471	1.00	36.17	A
	ATOM	121	CA	LYS	A	18	69.897	71.473	70.972	1.00	35.91	A
	ATOM	122	CB	LYS	A	18	71.208	72.003	71.541	1.00	35.90	A
	ATOM	123	CG	LYS	A	18	72.397	71.086	71.239	1.00	36.70	A
	ATOM	124	CD	LYS	A	18	73.679	71.525	71.964	1.00	37.63	A
20	ATOM	125	CE	LYS	A	18	74.131	72.918	71.523	1.00	38.26	A
	ATOM	126	NZ	LYS	A	18	75.528	73.223	71.956	1.00	38.28	A
	ATOM	127	C	LYS	A	18	69.776	70.010	71.319	1.00	36.47	A
	ATOM	128	O	LYS	A	18	70.048	69.129	70.497	1.00	35.04	A
	ATOM	129	N	LYS	A	19	69.388	69.756	72.559	1.00	38.15	A
25	ATOM	130	CA	LYS	A	19	69.220	68.393	73.011	1.00	38.79	A
	ATOM	131	CB	LYS	A	19	68.733	68.374	74.456	1.00	39.52	A
	ATOM	132	CG	LYS	A	19	68.597	66.980	75.018	0.00	40.07	A
	ATOM	133	CD	LYS	A	19	68.074	66.996	76.439	0.00	40.81	A
	ATOM	134	CE	LYS	A	19	66.638	67.489	76.505	0.00	41.30	A
30	ATOM	135	NZ	LYS	A	19	66.086	67.373	77.885	0.00	41.65	A
	ATOM	136	C	LYS	A	19	68.202	67.734	72.084	1.00	38.59	A
	ATOM	137	O	LYS	A	19	68.508	66.734	71.445	1.00	39.10	A
	ATOM	138	N	ILE	A	20	67.004	68.304	71.984	1.00	37.46	A
	ATOM	139	CA	ILE	A	20	65.991	67.725	71.112	1.00	37.39	A
35	ATOM	140	CB	ILE	A	20	64.685	68.503	71.168	1.00	36.72	A
	ATOM	141	CG2	ILE	A	20	63.687	67.918	70.167	1.00	36.45	A
	ATOM	142	CG1	ILE	A	20	64.118	68.440	72.572	1.00	35.02	A
	ATOM	143	CD1	ILE	A	20	62.910	69.280	72.751	1.00	36.54	A
	ATOM	144	C	ILE	A	20	66.432	67.678	69.660	1.00	37.89	A
40	ATOM	145	O	ILE	A	20	66.157	66.718	68.954	1.00	38.16	A
	ATOM	146	N	ALA	A	21	67.125	68.717	69.218	1.00	39.24	A
	ATOM	147	CA	ALA	A	21	67.591	68.793	67.843	1.00	38.28	A
	ATOM	148	CB	ALA	A	21	68.197	70.154	67.570	1.00	38.24	A
	ATOM	149	C	ALA	A	21	68.609	67.719	67.589	1.00	38.38	A
45	ATOM	150	O	ALA	A	21	68.798	67.294	66.455	1.00	38.91	A
	ATOM	151	N	GLU	A	22	69.281	67.276	68.640	1.00	38.98	A
	ATOM	152	CA	GLU	A	22	70.280	66.242	68.449	1.00	39.28	A
	ATOM	153	CB	GLU	A	22	71.102	66.063	69.717	1.00	42.76	A
	ATOM	154	CG	GLU	A	22	72.116	67.162	69.962	1.00	47.53	A
50	ATOM	155	CD	GLU	A	22	72.856	66.948	71.259	1.00	50.36	A
	ATOM	156	OE1	GLU	A	22	73.381	65.827	71.444	1.00	50.70	A
	ATOM	157	OE2	GLU	A	22	72.907	67.891	72.089	1.00	52.73	A
	ATOM	158	C	GLU	A	22	69.666	64.913	68.021	1.00	37.58	A
	ATOM	159	O	GLU	A	22	70.391	63.955	67.805	1.00	37.40	A

	ATOM	160	N	ARG	A	23	68.342	64.850	67.890	1.00	36.03	A
	ATOM	161	CA	ARG	A	23	67.706	63.615	67.459	1.00	34.62	A
	ATOM	162	CB	ARG	A	23	66.200	63.765	67.306	1.00	33.59	A
	ATOM	163	CG	ARG	A	23	65.509	62.431	67.022	1.00	33.69	A
5	ATOM	164	CD	ARG	A	23	65.708	61.463	68.191	1.00	33.70	A
	ATOM	165	NE	ARG	A	23	64.457	61.196	68.901	1.00	34.45	A
	ATOM	166	CZ	ARG	A	23	64.360	60.622	70.100	1.00	33.77	A
	ATOM	167	NH1	ARG	A	23	65.447	60.243	70.764	1.00	34.73	A
	ATOM	168	NH2	ARG	A	23	63.164	60.414	70.633	1.00	29.73	A
10	ATOM	169	C	ARG	A	23	68.270	63.248	66.116	1.00	35.80	A
	ATOM	170	O	ARG	A	23	68.362	62.077	65.769	1.00	37.71	A
	ATOM	171	N	SER	A	24	68.629	64.266	65.345	1.00	37.45	A
	ATOM	172	CA	SER	A	24	69.208	64.072	64.018	1.00	37.69	A
	ATOM	173	CB	SER	A	24	69.047	65.344	63.187	1.00	36.12	A
15	ATOM	174	OG	SER	A	24	69.929	65.337	62.084	1.00	32.96	A
	ATOM	175	C	SER	A	24	70.686	63.729	64.127	1.00	38.12	A
	ATOM	176	O	SER	A	24	71.506	64.581	64.466	1.00	36.69	A
	ATOM	177	N	LEU	A	25	71.022	62.478	63.837	1.00	40.01	A
	ATOM	178	CA	LEU	A	25	72.409	62.036	63.901	1.00	42.65	A
20	ATOM	179	CB	LEU	A	25	72.534	60.580	63.436	1.00	43.67	A
	ATOM	180	CG	LEU	A	25	71.996	59.493	64.383	1.00	43.11	A
	ATOM	181	CD1	LEU	A	25	72.208	58.104	63.794	1.00	41.75	A
	ATOM	182	CD2	LEU	A	25	72.703	59.615	65.713	1.00	41.72	A
	ATOM	183	C	LEU	A	25	73.313	62.916	63.054	1.00	42.76	A
25	ATOM	184	O	LEU	A	25	74.475	63.112	63.394	1.00	42.58	A
	ATOM	185	N	LEU	A	26	72.779	63.442	61.954	1.00	44.29	A
	ATOM	186	CA	LEU	A	26	73.554	64.309	61.070	1.00	46.11	A
	ATOM	187	CB	LEU	A	26	72.701	64.742	59.875	1.00	46.16	A
	ATOM	188	CG	LEU	A	26	73.318	65.721	58.868	1.00	45.56	A
30	ATOM	189	CD1	LEU	A	26	74.571	65.123	58.268	1.00	44.90	A
	ATOM	190	CD2	LEU	A	26	72.303	66.050	57.774	1.00	45.90	A
	ATOM	191	C	LEU	A	26	73.992	65.524	61.866	1.00	47.66	A
	ATOM	192	O	LEU	A	26	75.140	65.962	61.770	1.00	47.34	A
	ATOM	193	N	LEU	A	27	73.060	66.055	62.655	1.00	50.27	A
35	ATOM	194	CA	LEU	A	27	73.312	67.212	63.508	1.00	52.62	A
	ATOM	195	CB	LEU	A	27	71.985	67.831	63.963	1.00	52.60	A
	ATOM	196	CG	LEU	A	27	72.112	68.911	65.046	1.00	52.80	A
	ATOM	197	CD1	LEU	A	27	72.872	70.114	64.501	1.00	52.04	A
	ATOM	198	CD2	LEU	A	27	70.729	69.314	65.513	1.00	52.96	A
40	ATOM	199	C	LEU	A	27	74.145	66.835	64.742	1.00	54.44	A
	ATOM	200	O	LEU	A	27	75.085	67.540	65.100	1.00	54.34	A
	ATOM	201	N	LYS	A	28	73.786	65.726	65.387	1.00	56.05	A
	ATOM	202	CA	LYS	A	28	74.491	65.255	66.574	1.00	57.53	A
	ATOM	203	CB	LYS	A	28	73.880	63.942	67.059	1.00	58.27	A
45	ATOM	204	CG	LYS	A	28	74.486	63.418	68.347	0.00	58.77	A
	ATOM	205	CD	LYS	A	28	73.864	62.093	68.750	0.00	59.35	A
	ATOM	206	CE	LYS	A	28	74.520	61.545	70.004	0.00	59.70	A
	ATOM	207	NZ	LYS	A	28	73.986	60.205	70.367	0.00	59.95	A
	ATOM	208	C	LYS	A	28	75.974	65.049	66.297	0.00	58.99	A
50	ATOM	209	O	LYS	A	28	76.811	65.183	67.191	0.00	58.95	A
	ATOM	210	N	ASN	A	29	76.290	64.716	65.052	1.00	60.36	A
	ATOM	211	CA	ASN	A	29	77.667	64.489	64.647	1.00	62.38	A
	ATOM	212	CB	ASN	A	29	77.729	63.509	63.484	1.00	63.15	A
	ATOM	213	CG	ASN	A	29	77.458	62.085	63.908	1.00	64.88	A

5	ATOM	214	OD1	ASN	A	29	77.410	61.185	63.068	1.00	67.16	A
	ATOM	215	ND2	ASN	A	29	77.285	61.865	65.215	1.00	64.20	A
	ATOM	216	C	ASN	A	29	78.326	65.778	64.227	1.00	63.19	A
	ATOM	217	O	ASN	A	29	79.547	65.852	64.106	1.00	63.26	A
	ATOM	218	N	TYR	A	30	77.514	66.797	63.993	1.00	64.46	A
10	ATOM	219	CA	TYR	A	30	78.049	68.083	63.583	1.00	65.53	A
	ATOM	220	CB	TYR	A	30	76.898	69.085	63.417	1.00	67.82	A
	ATOM	221	CG	TYR	A	30	77.127	70.172	62.379	1.00	68.70	A
	ATOM	222	CD1	TYR	A	30	77.416	69.853	61.050	1.00	68.47	A
	ATOM	223	CE1	TYR	A	30	77.595	70.854	60.092	1.00	69.31	A
15	ATOM	224	CD2	TYR	A	30	77.024	71.522	62.722	1.00	68.53	A
	ATOM	225	CE2	TYR	A	30	77.201	72.528	61.774	1.00	69.17	A
	ATOM	226	CZ	TYR	A	30	77.485	72.190	60.464	1.00	69.54	A
	ATOM	227	OH	TYR	A	30	77.651	73.191	59.534	1.00	69.67	A
	ATOM	228	C	TYR	A	30	79.043	68.550	64.658	1.00	65.21	A
20	ATOM	229	O	TYR	A	30	79.894	69.395	64.391	1.00	64.91	A
	ATOM	230	N	VAL	A	31	78.935	67.964	65.856	1.00	64.85	A
	ATOM	231	CA	VAL	A	31	79.786	68.271	67.019	1.00	62.98	A
	ATOM	232	CB	VAL	A	31	81.049	67.351	67.096	1.00	62.18	A
	ATOM	233	CG1	VAL	A	31	80.624	65.903	67.216	1.00	61.36	A
25	ATOM	234	CG2	VAL	A	31	81.961	67.562	65.882	1.00	60.58	A
	ATOM	235	C	VAL	A	31	80.256	69.712	67.123	1.00	62.08	A
	ATOM	236	O	VAL	A	31	80.624	70.168	68.203	1.00	60.74	A
	ATOM	237	N	ILE	A	45	76.524	76.394	65.711	1.00	42.05	A
	ATOM	238	CA	ILE	A	45	75.216	76.668	66.290	1.00	41.90	A
30	ATOM	239	CB	ILE	A	45	75.276	77.864	67.310	1.00	42.05	A
	ATOM	240	CG2	ILE	A	45	75.089	79.191	66.601	1.00	40.06	A
	ATOM	241	CG1	ILE	A	45	74.171	77.726	68.363	1.00	43.22	A
	ATOM	242	CD1	ILE	A	45	74.407	76.620	69.388	1.00	43.84	A
	ATOM	243	C	ILE	A	45	74.180	76.963	65.195	1.00	41.36	A
35	ATOM	244	O	ILE	A	45	73.021	77.252	65.488	1.00	41.48	A
	ATOM	245	N	VAL	A	46	74.592	76.918	63.933	1.00	39.64	A
	ATOM	246	CA	VAL	A	46	73.635	77.132	62.849	1.00	39.19	A
	ATOM	247	CB	VAL	A	46	73.675	78.579	62.293	1.00	37.60	A
	ATOM	248	CG1	VAL	A	46	72.665	78.729	61.166	1.00	35.40	A
40	ATOM	249	CG2	VAL	A	46	73.346	79.567	63.390	1.00	38.18	A
	ATOM	250	C	VAL	A	46	73.917	76.159	61.715	1.00	39.41	A
	ATOM	251	O	VAL	A	46	74.815	76.385	60.905	1.00	41.28	A
	ATOM	252	N	MSE	A	47	73.160	75.069	61.655	1.00	38.13	A
	ATOM	253	CA	MSE	A	47	73.390	74.093	60.606	1.00	37.60	A
45	ATOM	254	CB	MSE	A	47	73.419	72.680	61.169	1.00	40.79	A
	ATOM	255	CG	MSE	A	47	73.777	71.642	60.118	1.00	44.02	A
	ATOM	256	SE	MSE	A	47	73.314	69.875	60.679	1.00	50.37	A
	ATOM	257	CE	MSE	A	47	71.388	70.111	60.653	1.00	48.04	A
	ATOM	258	C	MSE	A	47	72.402	74.138	59.465	1.00	36.07	A
50	ATOM	259	O	MSE	A	47	71.195	74.213	59.670	1.00	36.45	A
	ATOM	260	N	PRO	A	48	72.917	74.093	58.229	1.00	34.97	A
	ATOM	261	CD	PRO	A	48	74.305	74.434	57.870	1.00	34.19	A
	ATOM	262	CA	PRO	A	48	72.066	74.128	57.040	1.00	34.14	A
	ATOM	263	CB	PRO	A	48	73.041	74.516	55.929	1.00	33.07	A
	ATOM	264	CG	PRO	A	48	74.103	75.290	56.654	1.00	33.93	A
	ATOM	265	C	PRO	A	48	71.369	72.806	56.729	1.00	33.52	A
	ATOM	266	O	PRO	A	48	71.922	71.727	56.946	1.00	32.95	A
	ATOM	267	N	VAL	A	49	70.140	72.906	56.231	1.00	32.78	A

	ATOM	268	CA	VAL	A	49	69.383	71.731	55.828	1.00	32.43	A
	ATOM	269	CB	VAL	A	49	68.073	71.538	56.671	1.00	31.33	A
	ATOM	270	CG1	VAL	A	49	67.575	70.120	56.539	1.00	30.50	A
	ATOM	271	CG2	VAL	A	49	68.327	71.845	58.141	1.00	34.13	A
5	ATOM	272	C	VAL	A	49	69.062	71.991	54.340	1.00	32.95	A
	ATOM	273	O	VAL	A	49	67.958	72.412	53.977	1.00	32.24	A
	ATOM	274	N	PRO	A	50	70.060	71.757	53.460	1.00	33.40	A
	ATOM	275	CD	PRO	A	50	71.393	71.237	53.811	1.00	33.34	A
	ATOM	276	CA	PRO	A	50	69.971	71.942	52.010	1.00	32.39	A
10	ATOM	277	CB	PRO	A	50	71.310	71.409	51.512	1.00	32.52	A
	ATOM	278	CG	PRO	A	50	72.217	71.682	52.627	1.00	33.15	A
	ATOM	279	C	PRO	A	50	68.813	71.229	51.343	1.00	31.05	A
	ATOM	280	O	PRO	A	50	68.509	70.079	51.648	1.00	31.50	A
	ATOM	281	N	ASN	A	51	68.176	71.936	50.420	1.00	30.37	A
15	ATOM	282	CA	ASN	A	51	67.071	71.387	49.645	1.00	30.66	A
	ATOM	283	CB	ASN	A	51	67.648	70.432	48.595	1.00	31.76	A
	ATOM	284	CG	ASN	A	51	69.069	70.813	48.175	1.00	30.85	A
	ATOM	285	OD1	ASN	A	51	69.262	71.794	47.478	1.00	27.98	A
	ATOM	286	ND2	ASN	A	51	70.072	70.031	48.620	1.00	33.14	A
20	ATOM	287	C	ASN	A	51	65.978	70.665	50.450	1.00	29.20	A
	ATOM	288	O	ASN	A	51	65.588	69.551	50.120	1.00	26.62	A
	ATOM	289	N	VAL	A	52	65.500	71.292	51.512	1.00	29.33	A
	ATOM	290	CA	VAL	A	52	64.435	70.692	52.283	1.00	29.38	A
	ATOM	291	CB	VAL	A	52	64.913	70.157	53.640	1.00	30.20	A
25	ATOM	292	CG1	VAL	A	52	63.747	69.506	54.390	1.00	26.29	A
	ATOM	293	CG2	VAL	A	52	66.022	69.129	53.420	1.00	29.10	A
	ATOM	294	C	VAL	A	52	63.401	71.774	52.492	1.00	29.83	A
	ATOM	295	O	VAL	A	52	63.693	72.821	53.058	1.00	29.62	A
	ATOM	296	N	ARG	A	53	62.199	71.504	51.992	1.00	30.70	A
30	ATOM	297	CA	ARG	A	53	61.064	72.411	52.063	1.00	31.16	A
	ATOM	298	CB	ARG	A	53	59.814	71.667	51.580	1.00	35.30	A
	ATOM	299	CG	ARG	A	53	58.775	72.499	50.846	1.00	39.79	A
	ATOM	300	CD	ARG	A	53	57.564	71.636	50.474	1.00	42.92	A
	ATOM	301	NE	ARG	A	53	56.700	72.283	49.491	1.00	47.91	A
35	ATOM	302	CZ	ARG	A	53	55.889	73.308	49.749	1.00	50.95	A
	ATOM	303	NH1	ARG	A	53	55.815	73.814	50.972	1.00	53.87	A
	ATOM	304	NH2	ARG	A	53	55.158	73.844	48.776	1.00	52.85	A
	ATOM	305	C	ARG	A	53	60.864	72.876	53.505	1.00	30.38	A
	ATOM	306	O	ARG	A	53	60.860	72.068	54.425	1.00	31.84	A
40	ATOM	307	N	SER	A	54	60.694	74.173	53.708	1.00	27.65	A
	ATOM	308	CA	SER	A	54	60.481	74.670	55.050	1.00	24.25	A
	ATOM	309	CB	SER	A	54	60.094	76.142	55.013	1.00	23.48	A
	ATOM	310	OG	SER	A	54	61.197	76.935	54.642	1.00	22.07	A
	ATOM	311	C	SER	A	54	59.386	73.866	55.742	1.00	22.74	A
45	ATOM	312	O	SER	A	54	59.611	73.280	56.792	1.00	21.74	A
	ATOM	313	N	SER	A	55	58.204	73.835	55.143	1.00	22.72	A
	ATOM	314	CA	SER	A	55	57.078	73.114	55.707	1.00	22.82	A
	ATOM	315	CB	SER	A	55	55.913	73.117	54.736	1.00	20.88	A
	ATOM	316	OG	SER	A	55	56.159	72.211	53.683	1.00	23.15	A
50	ATOM	317	C	SER	A	55	57.432	71.670	56.042	1.00	24.40	A
	ATOM	318	O	SER	A	55	56.780	71.034	56.877	1.00	27.21	A
	ATOM	319	N	VAL	A	56	58.457	71.144	55.387	1.00	21.45	A
	ATOM	320	CA	VAL	A	56	58.862	69.782	55.662	1.00	20.79	A
	ATOM	321	CB	VAL	A	56	59.648	69.194	54.488	1.00	19.14	A

5	ATOM	322	CG1	VAL	A	56	60.254	67.875	54.889	1.00	16.99	A
	ATOM	323	CG2	VAL	A	56	58.738	69.029	53.301	1.00	18.04	A
	ATOM	324	C	VAL	A	56	59.719	69.727	56.924	1.00	21.47	A
	ATOM	325	O	VAL	A	56	59.498	68.903	57.797	1.00	21.73	A
	ATOM	326	N	LEU	A	57	60.703	70.606	57.010	1.00	22.90	A
10	ATOM	327	CA	LEU	A	57	61.573	70.645	58.159	1.00	24.53	A
	ATOM	328	CB	LEU	A	57	62.647	71.696	57.937	1.00	24.08	A
	ATOM	329	CG	LEU	A	57	63.681	71.859	59.042	1.00	24.59	A
	ATOM	330	CD1	LEU	A	57	64.030	70.523	59.664	1.00	23.09	A
	ATOM	331	CD2	LEU	A	57	64.924	72.530	58.438	1.00	23.83	A
15	ATOM	332	C	LEU	A	57	60.760	70.949	59.411	1.00	27.00	A
	ATOM	333	O	LEU	A	57	61.044	70.424	60.486	1.00	27.31	A
	ATOM	334	N	GLN	A	58	59.740	71.790	59.270	1.00	28.60	A
	ATOM	335	CA	GLN	A	58	58.885	72.133	60.402	1.00	29.92	A
	ATOM	336	CB	GLN	A	58	57.789	73.112	59.979	1.00	29.50	A
20	ATOM	337	CG	GLN	A	58	56.729	73.358	61.044	1.00	29.08	A
	ATOM	338	CD	GLN	A	58	55.975	74.654	60.815	1.00	27.90	A
	ATOM	339	OE1	GLN	A	58	56.591	75.700	60.657	1.00	30.17	A
	ATOM	340	NE2	GLN	A	58	54.648	74.594	60.802	1.00	25.55	A
	ATOM	341	C	GLN	A	58	58.257	70.845	60.886	1.00	30.93	A
25	ATOM	342	O	GLN	A	58	58.354	70.483	62.065	1.00	33.35	A
	ATOM	343	N	LYS	A	59	57.609	70.156	59.955	1.00	30.29	A
	ATOM	344	CA	LYS	A	59	56.976	68.880	60.248	1.00	29.48	A
	ATOM	345	CB	LYS	A	59	56.581	68.209	58.937	1.00	28.21	A
	ATOM	346	CG	LYS	A	59	55.283	67.470	58.978	1.00	29.03	A
30	ATOM	347	CD	LYS	A	59	54.108	68.397	59.081	1.00	27.32	A
	ATOM	348	CE	LYS	A	59	52.834	67.608	58.857	1.00	26.80	A
	ATOM	349	NZ	LYS	A	59	52.804	66.508	59.824	1.00	25.00	A
	ATOM	350	C	LYS	A	59	58.004	68.017	61.006	1.00	29.46	A
	ATOM	351	O	LYS	A	59	57.709	67.465	62.070	1.00	29.02	A
35	ATOM	352	N	VAL	A	60	59.217	67.929	60.467	1.00	28.15	A
	ATOM	353	CA	VAL	A	60	60.259	67.142	61.106	1.00	28.14	A
	ATOM	354	CB	VAL	A	60	61.573	67.226	60.319	1.00	28.15	A
	ATOM	355	CG1	VAL	A	60	62.731	66.715	61.152	1.00	27.46	A
	ATOM	356	CG2	VAL	A	60	61.455	66.386	59.060	1.00	29.05	A
40	ATOM	357	C	VAL	A	60	60.495	67.574	62.543	1.00	28.57	A
	ATOM	358	O	VAL	A	60	60.434	66.762	63.465	1.00	29.28	A
	ATOM	359	N	ILE	A	61	60.768	68.853	62.734	1.00	28.79	A
	ATOM	360	CA	ILE	A	61	61.007	69.375	64.068	1.00	28.54	A
	ATOM	361	CB	ILE	A	61	61.195	70.903	64.001	1.00	27.31	A
45	ATOM	362	CG2	ILE	A	61	61.238	71.501	65.391	1.00	26.36	A
	ATOM	363	CG1	ILE	A	61	62.482	71.202	63.223	1.00	27.68	A
	ATOM	364	CD1	ILE	A	61	62.737	72.660	62.979	1.00	27.54	A
	ATOM	365	C	ILE	A	61	59.860	69.020	65.016	1.00	29.35	A
	ATOM	366	O	ILE	A	61	60.086	68.538	66.131	1.00	27.58	A
50	ATOM	367	N	GLU	A	62	58.627	69.247	64.572	1.00	30.00	A
	ATOM	368	CA	GLU	A	62	57.473	68.949	65.415	1.00	31.73	A
	ATOM	369	CB	GLU	A	62	56.169	69.203	64.667	1.00	29.92	A
	ATOM	370	CG	GLU	A	62	55.043	68.328	65.181	1.00	30.57	A
	ATOM	371	CD	GLU	A	62	53.688	68.775	64.703	1.00	31.86	A
	ATOM	372	OE1	GLU	A	62	53.530	68.966	63.470	1.00	33.09	A
	ATOM	373	OE2	GLU	A	62	52.781	68.934	65.562	1.00	31.63	A
	ATOM	374	C	GLU	A	62	57.480	67.505	65.907	1.00	32.78	A
	ATOM	375	O	GLU	A	62	57.035	67.207	67.017	1.00	32.73	A

	ATOM	376	N	TRP	A	63	57.965	66.610	65.057	1.00	34.15	A
	ATOM	377	CA	TRP	A	63	58.029	65.204	65.394	1.00	34.37	A
	ATOM	378	CB	TRP	A	63	58.259	64.380	64.127	1.00	33.74	A
	ATOM	379	CG	TRP	A	63	58.189	62.915	64.354	1.00	31.94	A
5	ATOM	380	CD2	TRP	A	63	59.254	62.071	64.798	1.00	30.34	A
	ATOM	381	CE2	TRP	A	63	58.729	60.775	64.937	1.00	29.79	A
	ATOM	382	CE3	TRP	A	63	60.601	62.287	65.104	1.00	29.39	A
	ATOM	383	CD1	TRP	A	63	57.092	62.120	64.235	1.00	31.15	A
	ATOM	384	NE1	TRP	A	63	57.406	60.829	64.584	1.00	30.29	A
10	ATOM	385	CZ2	TRP	A	63	59.506	59.698	65.361	1.00	29.60	A
	ATOM	386	CZ3	TRP	A	63	61.372	61.211	65.528	1.00	28.85	A
	ATOM	387	CH2	TRP	A	63	60.821	59.937	65.654	1.00	27.95	A
	ATOM	388	C	TRP	A	63	59.181	64.989	66.372	1.00	34.92	A
	ATOM	389	O	TRP	A	63	59.146	64.078	67.182	1.00	36.00	A
15	ATOM	390	N	ALA	A	64	60.195	65.840	66.316	1.00	35.06	A
	ATOM	391	CA	ALA	A	64	61.332	65.673	67.207	1.00	36.52	A
	ATOM	392	CB	ALA	A	64	62.567	66.371	66.621	1.00	35.61	A
	ATOM	393	C	ALA	A	64	61.071	66.166	68.636	1.00	38.06	A
	ATOM	394	O	ALA	A	64	61.606	65.607	69.602	1.00	38.15	A
20	ATOM	395	N	GLU	A	65	60.266	67.218	68.764	1.00	38.68	A
	ATOM	396	CA	GLU	A	65	59.934	67.776	70.063	1.00	38.24	A
	ATOM	397	CB	GLU	A	65	59.405	69.201	69.912	1.00	38.18	A
	ATOM	398	CG	GLU	A	65	60.459	70.151	69.397	1.00	38.80	A
	ATOM	399	CD	GLU	A	65	59.895	71.454	68.840	1.00	39.78	A
25	ATOM	400	OE1	GLU	A	65	58.673	71.527	68.547	1.00	38.29	A
	ATOM	401	OE2	GLU	A	65	60.695	72.408	68.683	1.00	39.80	A
	ATOM	402	C	GLU	A	65	58.879	66.902	70.708	1.00	38.37	A
	ATOM	403	O	GLU	A	65	58.835	66.742	71.925	1.00	39.26	A
	ATOM	404	N	HIS	A	66	58.024	66.312	69.896	1.00	38.38	A
30	ATOM	405	CA	HIS	A	66	57.006	65.482	70.479	1.00	40.16	A
	ATOM	406	CB	HIS	A	66	55.929	65.179	69.465	1.00	39.56	A
	ATOM	407	CG	HIS	A	66	54.902	64.215	69.955	1.00	39.86	A
	ATOM	408	CD2	HIS	A	66	53.613	64.399	70.320	1.00	39.39	A
	ATOM	409	ND1	HIS	A	66	55.137	62.859	70.036	1.00	38.45	A
35	ATOM	410	CE1	HIS	A	66	54.031	62.248	70.418	1.00	38.21	A
	ATOM	411	NE2	HIS	A	66	53.091	63.159	70.595	1.00	39.69	A
	ATOM	412	C	HIS	A	66	57.616	64.205	71.002	1.00	42.15	A
	ATOM	413	O	HIS	A	66	57.115	63.619	71.959	1.00	44.74	A
	ATOM	414	N	HIS	A	67	58.701	63.775	70.377	1.00	43.11	A
40	ATOM	415	CA	HIS	A	67	59.388	62.573	70.807	1.00	44.64	A
	ATOM	416	CB	HIS	A	67	59.711	61.681	69.598	1.00	43.57	A
	ATOM	417	CG	HIS	A	67	58.524	60.951	69.046	1.00	42.88	A
	ATOM	418	CD2	HIS	A	67	58.088	59.684	69.241	1.00	42.35	A
	ATOM	419	ND1	HIS	A	67	57.615	61.540	68.194	1.00	43.39	A
45	ATOM	420	CE1	HIS	A	67	56.673	60.667	67.886	1.00	41.93	A
	ATOM	421	NE2	HIS	A	67	56.936	59.533	68.508	1.00	40.92	A
	ATOM	422	C	HIS	A	67	60.673	62.989	71.512	1.00	46.18	A
	ATOM	423	O	HIS	A	67	61.767	62.552	71.144	1.00	47.55	A
	ATOM	424	N	ARG	A	68	60.541	63.842	72.524	1.00	47.19	A
50	ATOM	425	CA	ARG	A	68	61.704	64.322	73.270	1.00	48.05	A
	ATOM	426	CB	ARG	A	68	61.390	65.665	73.959	1.00	47.55	A
	ATOM	427	CG	ARG	A	68	60.459	65.576	75.163	1.00	47.12	A
	ATOM	428	CD	ARG	A	68	60.219	66.943	75.813	1.00	45.40	A
	ATOM	429	NE	ARG	A	68	59.137	67.657	75.151	1.00	44.72	A

	ATOM	430	CZ	ARG	A	68	57.849	67.387	75.342	1.00	44.29	A
	ATOM	431	NH1	ARG	A	68	57.485	66.434	76.179	1.00	46.93	A
	ATOM	432	NH2	ARG	A	68	56.915	68.043	74.678	1.00	45.61	A
	ATOM	433	C	ARG	A	68	62.187	63.308	74.303	1.00	49.19	A
5	ATOM	434	O	ARG	A	68	63.383	63.228	74.593	1.00	48.48	A
	ATOM	435	N	ASP	A	69	61.261	62.525	74.848	1.00	51.12	A
	ATOM	436	CA	ASP	A	69	61.626	61.531	75.853	1.00	52.05	A
	ATOM	437	CB	ASP	A	69	60.967	61.862	77.187	1.00	50.12	A
	ATOM	438	CG	ASP	A	69	61.351	63.221	77.684	1.00	49.36	A
10	ATOM	439	OD1	ASP	A	69	62.572	63.496	77.736	1.00	48.50	A
	ATOM	440	OD2	ASP	A	69	60.440	64.010	78.015	1.00	49.39	A
	ATOM	441	C	ASP	A	69	61.245	60.126	75.442	1.00	52.86	A
	ATOM	442	O	ASP	A	69	60.787	59.335	76.261	1.00	52.94	A
	ATOM	443	N	SER	A	70	61.437	59.812	74.170	1.00	54.02	A
15	ATOM	444	CA	SER	A	70	61.106	58.488	73.690	1.00	55.97	A
	ATOM	445	CB	SER	A	70	60.259	58.588	72.425	1.00	54.70	A
	ATOM	446	OG	SER	A	70	59.031	59.239	72.703	1.00	54.60	A
	ATOM	447	C	SER	A	70	62.379	57.702	73.425	1.00	58.22	A
	ATOM	448	O	SER	A	70	63.463	58.273	73.306	1.00	58.71	A
20	ATOM	449	N	ASN	A	71	62.252	56.385	73.362	1.00	60.80	A
	ATOM	450	CA	ASN	A	71	63.403	55.545	73.105	1.00	64.11	A
	ATOM	451	CB	ASN	A	71	63.999	55.049	74.421	1.00	62.74	A
	ATOM	452	CG	ASN	A	71	64.012	56.121	75.495	1.00	62.42	A
	ATOM	453	OD1	ASN	A	71	63.016	56.332	76.183	1.00	61.70	A
25	ATOM	454	ND2	ASN	A	71	65.139	56.811	75.636	1.00	62.41	A
	ATOM	455	C	ASN	A	71	62.957	54.377	72.247	1.00	67.50	A
	ATOM	456	O	ASN	A	71	62.140	53.558	72.669	1.00	68.91	A
	ATOM	457	N	PHE	A	72	63.486	54.313	71.030	1.00	70.54	A
	ATOM	458	CA	PHE	A	72	63.134	53.245	70.110	1.00	72.15	A
30	ATOM	459	CB	PHE	A	72	62.792	53.827	68.721	1.00	72.15	A
	ATOM	460	CG	PHE	A	72	61.940	55.087	68.759	1.00	71.12	A
	ATOM	461	CD1	PHE	A	72	62.539	56.349	68.784	1.00	70.74	A
	ATOM	462	CD2	PHE	A	72	60.546	55.012	68.765	1.00	70.32	A
	ATOM	463	CE1	PHE	A	72	61.767	57.514	68.814	1.00	70.31	A
35	ATOM	464	CE2	PHE	A	72	59.768	56.173	68.796	1.00	70.64	A
	ATOM	465	CZ	PHE	A	72	60.383	57.425	68.821	1.00	70.21	A
	ATOM	466	C	PHE	A	72	64.307	52.261	70.001	1.00	73.60	A
	ATOM	467	O	PHE	A	72	65.466	52.623	70.226	1.00	73.93	A
	ATOM	468	N	PRO	A	73	64.012	50.992	69.685	1.00	75.25	A
40	ATOM	469	CD	PRO	A	73	62.656	50.410	69.635	1.00	75.90	A
	ATOM	470	CA	PRO	A	73	65.039	49.952	69.545	1.00	75.83	A
	ATOM	471	CB	PRO	A	73	64.230	48.732	69.122	1.00	76.63	A
	ATOM	472	CG	PRO	A	73	62.924	48.937	69.852	1.00	76.34	A
	ATOM	473	C	PRO	A	73	66.099	50.325	68.511	0.00	76.16	A
45	ATOM	474	O	PRO	A	73	67.292	50.365	68.813	0.00	76.37	A
	ATOM	475	N	VAL	A	86	52.596	52.678	63.351	1.00	68.06	A
	ATOM	476	CA	VAL	A	86	52.119	51.882	64.474	1.00	69.23	A
	ATOM	477	CB	VAL	A	86	53.259	50.998	65.073	1.00	69.13	A
	ATOM	478	CG1	VAL	A	86	52.716	50.130	66.203	1.00	68.76	A
50	ATOM	479	CG2	VAL	A	86	53.864	50.111	63.989	1.00	69.85	A
	ATOM	480	C	VAL	A	86	51.576	52.809	65.562	1.00	69.62	A
	ATOM	481	O	VAL	A	86	50.459	52.627	66.061	1.00	69.53	A
	ATOM	482	N	ASP	A	87	52.368	53.821	65.907	1.00	69.73	A
	ATOM	483	CA	ASP	A	87	51.995	54.792	66.936	1.00	68.97	A

5	ATOM	484	CB	ASP	A	87	53.177	55.726	67.223	1.00	70.05	A
	ATOM	485	CG	ASP	A	87	52.982	56.555	68.487	1.00	70.55	A
	ATOM	486	OD1	ASP	A	87	52.047	57.386	68.514	1.00	70.97	A
	ATOM	487	OD2	ASP	A	87	53.768	56.374	69.447	1.00	69.47	A
	ATOM	488	C	ASP	A	87	50.766	55.609	66.528	1.00	67.85	A
10	ATOM	489	O	ASP	A	87	50.574	55.925	65.353	1.00	67.51	A
	ATOM	490	N	SER	A	88	49.936	55.948	67.510	1.00	66.47	A
	ATOM	491	CA	SER	A	88	48.714	56.708	67.263	1.00	64.69	A
	ATOM	492	CB	SER	A	88	47.872	56.772	68.537	1.00	65.29	A
	ATOM	493	OG	SER	A	88	46.724	57.579	68.337	1.00	66.37	A
15	ATOM	494	C	SER	A	88	48.976	58.124	66.770	1.00	62.66	A
	ATOM	495	O	SER	A	88	48.420	58.553	65.755	1.00	61.70	A
	ATOM	496	N	TRP	A	89	49.824	58.843	67.498	1.00	60.57	A
	ATOM	497	CA	TRP	A	89	50.161	60.221	67.160	1.00	58.68	A
	ATOM	498	CB	TRP	A	89	50.999	60.836	68.281	1.00	57.33	A
20	ATOM	499	CG	TRP	A	89	51.130	62.296	68.148	1.00	56.37	A
	ATOM	500	CD2	TRP	A	89	52.229	62.998	67.571	1.00	56.15	A
	ATOM	501	CE2	TRP	A	89	51.892	64.365	67.574	1.00	55.64	A
	ATOM	502	CE3	TRP	A	89	53.463	62.605	67.044	1.00	55.77	A
	ATOM	503	CD1	TRP	A	89	50.201	63.231	68.477	1.00	54.82	A
25	ATOM	504	NE1	TRP	A	89	50.649	64.480	68.136	1.00	54.93	A
	ATOM	505	CZ2	TRP	A	89	52.755	65.342	67.072	1.00	55.82	A
	ATOM	506	CZ3	TRP	A	89	54.315	63.579	66.544	1.00	55.23	A
	ATOM	507	CH2	TRP	A	89	53.957	64.927	66.561	1.00	55.54	A
	ATOM	508	C	TRP	A	89	50.915	60.332	65.831	1.00	57.32	A
30	ATOM	509	O	TRP	A	89	50.679	61.248	65.045	1.00	57.65	A
	ATOM	510	N	ASP	A	90	51.827	59.398	65.593	1.00	55.46	A
	ATOM	511	CA	ASP	A	90	52.602	59.387	64.366	1.00	53.21	A
	ATOM	512	CB	ASP	A	90	53.710	58.353	64.472	1.00	51.45	A
	ATOM	513	CG	ASP	A	90	54.795	58.795	65.396	1.00	51.44	A
35	ATOM	514	OD1	ASP	A	90	54.462	59.439	66.401	1.00	53.33	A
	ATOM	515	OD2	ASP	A	90	55.975	58.511	65.134	1.00	51.16	A
	ATOM	516	C	ASP	A	90	51.731	59.082	63.162	1.00	53.01	A
	ATOM	517	O	ASP	A	90	51.943	59.625	62.076	1.00	53.15	A
	ATOM	518	N	ARG	A	91	50.746	58.214	63.362	1.00	52.99	A
40	ATOM	519	CA	ARG	A	91	49.835	57.822	62.293	1.00	52.82	A
	ATOM	520	CB	ARG	A	91	48.865	56.747	62.802	1.00	53.81	A
	ATOM	521	CG	ARG	A	91	47.856	56.264	61.770	1.00	56.18	A
	ATOM	522	CD	ARG	A	91	47.412	54.828	62.031	1.00	58.29	A
	ATOM	523	NE	ARG	A	91	46.995	54.617	63.412	1.00	61.35	A
45	ATOM	524	CZ	ARG	A	91	45.922	55.168	63.972	1.00	62.36	A
	ATOM	525	NH1	ARG	A	91	45.138	55.972	63.267	1.00	64.03	A
	ATOM	526	NH2	ARG	A	91	45.640	54.925	65.246	1.00	63.29	A
	ATOM	527	C	ARG	A	91	49.065	59.014	61.728	1.00	51.91	A
	ATOM	528	O	ARG	A	91	48.829	59.086	60.522	1.00	51.24	A
50	ATOM	529	N	GLU	A	92	48.683	59.946	62.599	1.00	50.83	A
	ATOM	530	CA	GLU	A	92	47.955	61.136	62.172	1.00	50.40	A
	ATOM	531	CB	GLU	A	92	47.181	61.750	63.337	1.00	52.44	A
	ATOM	532	CG	GLU	A	92	46.026	60.914	63.856	1.00	58.05	A
	ATOM	533	CD	GLU	A	92	44.989	60.594	62.787	1.00	60.95	A
	ATOM	534	OE1	GLU	A	92	44.493	61.541	62.125	1.00	61.85	A
	ATOM	535	OE2	GLU	A	92	44.670	59.392	62.621	1.00	61.47	A
	ATOM	536	C	GLU	A	92	48.929	62.174	61.632	1.00	48.17	A
	ATOM	537	O	GLU	A	92	48.689	62.784	60.589	1.00	48.86	A

	ATOM	538	N	PHE	A	93	50.020	62.376	62.364	1.00	45.11	A
	ATOM	539	CA	PHE	A	93	51.056	63.325	61.989	1.00	42.22	A
	ATOM	540	CB	PHE	A	93	52.241	63.197	62.930	1.00	39.86	A
	ATOM	541	CG	PHE	A	93	53.473	63.881	62.431	1.00	38.61	A
5	ATOM	542	CD1	PHE	A	93	53.560	65.270	62.434	1.00	38.78	A
	ATOM	543	CD2	PHE	A	93	54.550	63.139	61.949	1.00	38.41	A
	ATOM	544	CE1	PHE	A	93	54.706	65.920	61.962	1.00	37.98	A
	ATOM	545	CE2	PHE	A	93	55.702	63.771	61.474	1.00	37.53	A
	ATOM	546	CZ	PHE	A	93	55.782	65.169	61.482	1.00	37.66	A
10	ATOM	547	C	PHE	A	93	51.529	63.039	60.586	1.00	41.92	A
	ATOM	548	O	PHE	A	93	51.915	63.940	59.847	1.00	42.62	A
	ATOM	549	N	LEU	A	94	51.513	61.766	60.229	1.00	41.18	A
	ATOM	550	CA	LEU	A	94	51.938	61.368	58.913	1.00	40.65	A
	ATOM	551	CB	LEU	A	94	52.602	60.008	58.986	1.00	39.81	A
15	ATOM	552	CG	LEU	A	94	53.987	60.082	59.611	1.00	40.12	A
	ATOM	553	CD1	LEU	A	94	54.560	58.682	59.692	1.00	40.00	A
	ATOM	554	CD2	LEU	A	94	54.889	60.998	58.785	1.00	38.29	A
	ATOM	555	C	LEU	A	94	50.792	61.333	57.927	1.00	41.17	A
	ATOM	556	O	LEU	A	94	51.010	61.120	56.737	1.00	41.27	A
20	ATOM	557	N	LYS	A	95	49.575	61.553	58.413	1.00	41.25	A
	ATOM	558	CA	LYS	A	95	48.420	61.534	57.532	1.00	42.22	A
	ATOM	559	CB	LYS	A	95	47.120	61.460	58.342	1.00	43.14	A
	ATOM	560	CG	LYS	A	95	45.925	61.168	57.438	1.00	47.48	A
	ATOM	561	CD	LYS	A	95	44.586	61.331	58.138	1.00	51.30	A
25	ATOM	562	CE	LYS	A	95	44.392	60.305	59.252	1.00	53.68	A
	ATOM	563	NZ	LYS	A	95	43.042	60.431	59.895	1.00	54.53	A
	ATOM	564	C	LYS	A	95	48.390	62.762	56.616	1.00	41.83	A
	ATOM	565	O	LYS	A	95	47.450	63.552	56.650	1.00	42.87	A
	ATOM	566	N	VAL	A	96	49.406	62.890	55.770	1.00	41.34	A
30	ATOM	567	CA	VAL	A	96	49.545	64.023	54.856	1.00	40.71	A
	ATOM	568	CB	VAL	A	96	50.909	64.673	55.057	1.00	40.36	A
	ATOM	569	CG1	VAL	A	96	51.034	65.180	56.471	1.00	39.98	A
	ATOM	570	CG2	VAL	A	96	51.990	63.651	54.777	1.00	38.65	A
	ATOM	571	C	VAL	A	96	49.446	63.611	53.385	1.00	41.10	A
35	ATOM	572	O	VAL	A	96	49.074	62.482	53.077	1.00	39.99	A
	ATOM	573	N	ASP	A	97	49.789	64.518	52.471	1.00	41.74	A
	ATOM	574	CA	ASP	A	97	49.729	64.155	51.064	1.00	43.35	A
	ATOM	575	CB	ASP	A	97	49.500	65.386	50.168	1.00	46.03	A
	ATOM	576	CG	ASP	A	97	50.694	66.307	50.088	1.00	49.27	A
40	ATOM	577	OD1	ASP	A	97	51.762	65.862	49.621	1.00	51.92	A
	ATOM	578	OD2	ASP	A	97	50.560	67.490	50.476	1.00	50.75	A
	ATOM	579	C	ASP	A	97	50.976	63.369	50.642	1.00	42.71	A
	ATOM	580	O	ASP	A	97	52.039	63.493	51.249	1.00	42.39	A
	ATOM	581	N	GLN	A	98	50.815	62.549	49.606	1.00	41.92	A
45	ATOM	582	CA	GLN	A	98	51.867	61.690	49.097	1.00	40.58	A
	ATOM	583	CB	GLN	A	98	51.392	60.988	47.807	1.00	42.66	A
	ATOM	584	CG	GLN	A	98	49.949	60.414	47.882	1.00	43.12	A
	ATOM	585	CD	GLN	A	98	49.666	59.270	46.905	1.00	43.62	A
	ATOM	586	OE1	GLN	A	98	48.516	58.876	46.720	1.00	42.97	A
50	ATOM	587	NE2	GLN	A	98	50.712	58.732	46.290	1.00	44.27	A
	ATOM	588	C	GLN	A	98	53.173	62.428	48.870	1.00	39.89	A
	ATOM	589	O	GLN	A	98	54.234	61.905	49.180	1.00	38.30	A
	ATOM	590	N	GLU	A	99	53.114	63.640	48.330	1.00	40.88	A
	ATOM	591	CA	GLU	A	99	54.343	64.404	48.118	1.00	40.74	A

	ATOM	592	CB	GLU	A	99	54.035	65.695	47.377	1.00	41.69	A
	ATOM	593	CG	GLU	A	99	53.880	65.494	45.903	1.00	47.00	A
	ATOM	594	CD	GLU	A	99	55.182	65.074	45.254	1.00	48.98	A
	ATOM	595	OE1	GLU	A	99	56.236	65.569	45.721	1.00	50.30	A
5	ATOM	596	OE2	GLU	A	99	55.154	64.274	44.284	1.00	48.68	A
	ATOM	597	C	GLU	A	99	54.984	64.710	49.474	1.00	39.87	A
	ATOM	598	O	GLU	A	99	56.164	64.426	49.691	1.00	39.94	A
	ATOM	599	N	MSE	A	100	54.187	65.272	50.382	1.00	39.05	A
	ATOM	600	CA	MSE	A	100	54.637	65.617	51.729	1.00	39.03	A
10	ATOM	601	CB	MSE	A	100	53.434	66.000	52.603	1.00	45.07	A
	ATOM	602	CG	MSE	A	100	53.726	66.188	54.093	1.00	50.78	A
	ATOM	603	SE	MSE	A	100	54.480	67.900	54.500	1.00	61.41	A
	ATOM	604	CE	MSE	A	100	56.351	67.467	54.330	1.00	55.82	A
	ATOM	605	C	MSE	A	100	55.366	64.446	52.371	1.00	36.07	A
15	ATOM	606	O	MSE	A	100	56.517	64.561	52.789	1.00	34.98	A
	ATOM	607	N	LEU	A	101	54.681	63.316	52.436	1.00	32.38	A
	ATOM	608	CA	LEU	A	101	55.238	62.126	53.031	1.00	31.39	A
	ATOM	609	CB	LEU	A	101	54.241	60.993	52.880	1.00	30.22	A
	ATOM	610	CG	LEU	A	101	54.616	59.676	53.538	1.00	29.99	A
20	ATOM	611	CD1	LEU	A	101	54.859	59.906	55.028	1.00	29.67	A
	ATOM	612	CD2	LEU	A	101	53.501	58.674	53.287	1.00	26.62	A
	ATOM	613	C	LEU	A	101	56.571	61.745	52.394	1.00	31.59	A
	ATOM	614	O	LEU	A	101	57.523	61.341	53.077	1.00	32.03	A
	ATOM	615	N	TYR	A	102	56.624	61.872	51.076	1.00	30.32	A
25	ATOM	616	CA	TYR	A	102	57.814	61.556	50.311	1.00	29.70	A
	ATOM	617	CB	TYR	A	102	57.550	61.840	48.838	1.00	29.09	A
	ATOM	618	CG	TYR	A	102	58.765	61.747	47.940	1.00	27.92	A
	ATOM	619	CD1	TYR	A	102	59.402	60.530	47.709	1.00	27.22	A
	ATOM	620	CE1	TYR	A	102	60.478	60.441	46.831	1.00	27.22	A
30	ATOM	621	CD2	TYR	A	102	59.243	62.873	47.274	1.00	26.92	A
	ATOM	622	CE2	TYR	A	102	60.314	62.792	46.401	1.00	24.90	A
	ATOM	623	CZ	TYR	A	102	60.921	61.580	46.181	1.00	26.49	A
	ATOM	624	OH	TYR	A	102	61.959	61.497	45.299	1.00	26.37	A
	ATOM	625	C	TYR	A	102	58.970	62.409	50.796	1.00	30.50	A
35	ATOM	626	O	TYR	A	102	60.057	61.905	51.125	1.00	30.28	A
	ATOM	627	N	GLU	A	103	58.731	63.715	50.839	1.00	31.34	A
	ATOM	628	CA	GLU	A	103	59.763	64.645	51.276	1.00	32.16	A
	ATOM	629	CB	GLU	A	103	59.314	66.088	50.966	1.00	32.79	A
	ATOM	630	CG	GLU	A	103	58.921	66.251	49.492	1.00	35.11	A
40	ATOM	631	CD	GLU	A	103	58.538	67.673	49.065	1.00	37.94	A
	ATOM	632	OE1	GLU	A	103	57.628	68.279	49.685	1.00	37.38	A
	ATOM	633	OE2	GLU	A	103	59.138	68.175	48.084	1.00	37.07	A
	ATOM	634	C	GLU	A	103	60.128	64.438	52.760	1.00	30.98	A
	ATOM	635	O	GLU	A	103	61.292	64.600	53.136	1.00	30.87	A
45	ATOM	636	N	ILE	A	104	59.159	64.038	53.588	1.00	29.27	A
	ATOM	637	CA	ILE	A	104	59.426	63.804	55.011	1.00	28.70	A
	ATOM	638	CB	ILE	A	104	58.113	63.589	55.813	1.00	28.55	A
	ATOM	639	CG2	ILE	A	104	58.424	62.958	57.189	1.00	29.44	A
	ATOM	640	CG1	ILE	A	104	57.396	64.942	55.975	1.00	26.70	A
50	ATOM	641	CD1	ILE	A	104	56.098	64.917	56.782	1.00	22.17	A
	ATOM	642	C	ILE	A	104	60.359	62.609	55.221	1.00	27.96	A
	ATOM	643	O	ILE	A	104	61.180	62.591	56.144	1.00	26.87	A
	ATOM	644	N	ILE	A	105	60.225	61.609	54.360	1.00	27.92	A
	ATOM	645	CA	ILE	A	105	61.082	60.439	54.435	1.00	26.71	A

	ATOM	646	CB	ILE	A	105	60.543	59.321	53.534	1.00	26.61	A
	ATOM	647	CG2	ILE	A	105	61.590	58.215	53.388	1.00	25.95	A
	ATOM	648	CG1	ILE	A	105	59.200	58.836	54.106	1.00	26.49	A
	ATOM	649	CD1	ILE	A	105	58.546	57.701	53.349	1.00	26.37	A
5	ATOM	650	C	ILE	A	105	62.500	60.825	54.017	1.00	26.46	A
	ATOM	651	O	ILE	A	105	63.484	60.401	54.639	1.00	26.10	A
	ATOM	652	N	LEU	A	106	62.603	61.648	52.975	1.00	25.01	A
	ATOM	653	CA	LEU	A	106	63.915	62.084	52.505	1.00	24.17	A
	ATOM	654	CB	LEU	A	106	63.802	62.917	51.230	1.00	23.30	A
10	ATOM	655	CG	LEU	A	106	63.211	62.283	49.961	1.00	22.86	A
	ATOM	656	CD1	LEU	A	106	63.415	63.252	48.829	1.00	19.46	A
	ATOM	657	CD2	LEU	A	106	63.875	60.950	49.639	1.00	17.99	A
	ATOM	658	C	LEU	A	106	64.612	62.904	53.574	1.00	24.05	A
	ATOM	659	O	LEU	A	106	65.792	62.701	53.860	1.00	24.80	A
15	ATOM	660	N	ALA	A	107	63.875	63.835	54.168	1.00	23.58	A
	ATOM	661	CA	ALA	A	107	64.430	64.676	55.218	1.00	23.64	A
	ATOM	662	CB	ALA	A	107	63.388	65.684	55.684	1.00	21.11	A
	ATOM	663	C	ALA	A	107	64.901	63.817	56.393	1.00	23.90	A
	ATOM	664	O	ALA	A	107	65.978	64.046	56.952	1.00	23.39	A
20	ATOM	665	N	ALA	A	108	64.093	62.838	56.779	1.00	24.83	A
	ATOM	666	CA	ALA	A	108	64.479	61.970	57.879	1.00	27.43	A
	ATOM	667	CB	ALA	A	108	63.343	60.984	58.215	1.00	27.65	A
	ATOM	668	C	ALA	A	108	65.727	61.211	57.456	1.00	28.80	A
	ATOM	669	O	ALA	A	108	66.646	61.009	58.249	1.00	29.92	A
25	ATOM	670	N	ASN	A	109	65.763	60.794	56.196	1.00	28.89	A
	ATOM	671	CA	ASN	A	109	66.920	60.062	55.719	1.00	29.68	A
	ATOM	672	CB	ASN	A	109	66.631	59.416	54.361	1.00	31.27	A
	ATOM	673	CG	ASN	A	109	67.744	58.480	53.915	1.00	31.80	A
	ATOM	674	OD1	ASN	A	109	68.755	58.912	53.362	1.00	31.60	A
30	ATOM	675	ND2	ASN	A	109	67.568	57.186	54.178	1.00	32.93	A
	ATOM	676	C	ASN	A	109	68.153	60.956	55.628	1.00	30.29	A
	ATOM	677	O	ASN	A	109	69.248	60.524	55.959	1.00	30.81	A
	ATOM	678	N	TYR	A	110	67.992	62.197	55.177	1.00	31.42	A
	ATOM	679	CA	TYR	A	110	69.133	63.105	55.080	1.00	31.10	A
35	ATOM	680	CB	TYR	A	110	68.756	64.363	54.312	1.00	29.98	A
	ATOM	681	CG	TYR	A	110	69.819	65.437	54.351	1.00	30.69	A
	ATOM	682	CD1	TYR	A	110	71.057	65.237	53.736	1.00	29.71	A
	ATOM	683	CE1	TYR	A	110	72.022	66.241	53.716	1.00	30.17	A
	ATOM	684	CD2	TYR	A	110	69.571	66.674	54.965	1.00	31.52	A
40	ATOM	685	CE2	TYR	A	110	70.526	67.686	54.954	1.00	31.71	A
	ATOM	686	CZ	TYR	A	110	71.750	67.463	54.318	1.00	32.53	A
	ATOM	687	OH	TYR	A	110	72.680	68.481	54.226	1.00	33.63	A
	ATOM	688	C	TYR	A	110	69.620	63.515	56.463	1.00	31.73	A
	ATOM	689	O	TYR	A	110	70.818	63.603	56.694	1.00	32.81	A
45	ATOM	690	N	LEU	A	111	68.682	63.770	57.371	1.00	30.92	A
	ATOM	691	CA	LEU	A	111	69.016	64.184	58.719	1.00	31.21	A
	ATOM	692	CB	LEU	A	111	67.870	64.994	59.317	1.00	28.89	A
	ATOM	693	CG	LEU	A	111	67.630	66.380	58.734	1.00	26.61	A
	ATOM	694	CD1	LEU	A	111	66.251	66.831	59.141	1.00	24.78	A
50	ATOM	695	CD2	LEU	A	111	68.694	67.360	59.200	1.00	24.10	A
	ATOM	696	C	LEU	A	111	69.337	63.006	59.624	1.00	33.12	A
	ATOM	697	O	LEU	A	111	69.590	63.181	60.816	1.00	34.02	A
	ATOM	698	N	ASN	A	112	69.319	61.805	59.062	1.00	33.71	A
	ATOM	699	CA	ASN	A	112	69.620	60.588	59.820	1.00	34.83	A

	ATOM	700	CB	ASN	A	112	71.102	60.570	60.204	1.00	33.95	A
	ATOM	701	CG	ASN	A	112	71.644	59.164	60.365	1.00	33.26	A
	ATOM	702	OD1	ASN	A	112	71.015	58.322	60.977	1.00	34.03	A
	ATOM	703	ND2	ASN	A	112	72.820	58.913	59.813	1.00	34.72	A
5	ATOM	704	C	ASN	A	112	68.764	60.460	61.091	1.00	35.67	A
	ATOM	705	O	ASN	A	112	69.272	60.582	62.209	1.00	37.75	A
	ATOM	706	N	ILE	A	113	67.472	60.203	60.906	1.00	35.48	A
	ATOM	707	CA	ILE	A	113	66.517	60.055	62.005	1.00	35.39	A
	ATOM	708	CB	ILE	A	113	65.531	61.253	62.034	1.00	35.97	A
10	ATOM	709	CG2	ILE	A	113	64.563	61.125	63.200	1.00	35.08	A
	ATOM	710	CG1	ILE	A	113	66.307	62.567	62.154	1.00	36.19	A
	ATOM	711	CD1	ILE	A	113	65.427	63.795	62.132	1.00	33.68	A
	ATOM	712	C	ILE	A	113	65.738	58.761	61.763	1.00	35.67	A
	ATOM	713	O	ILE	A	113	64.564	58.789	61.381	1.00	33.98	A
15	ATOM	714	N	LYS	A	114	66.408	57.632	61.988	1.00	37.77	A
	ATOM	715	CA	LYS	A	114	65.827	56.299	61.775	1.00	39.09	A
	ATOM	716	CB	LYS	A	114	66.697	55.238	62.461	1.00	41.82	A
	ATOM	717	CG	LYS	A	114	67.835	54.703	61.601	1.00	45.96	A
	ATOM	718	CD	LYS	A	114	68.786	55.789	61.081	1.00	47.81	A
20	ATOM	719	CE	LYS	A	114	69.952	55.145	60.306	1.00	49.70	A
	ATOM	720	NZ	LYS	A	114	69.498	54.249	59.161	1.00	51.87	A
	ATOM	721	C	LYS	A	114	64.372	56.128	62.216	1.00	37.68	A
	ATOM	722	O	LYS	A	114	63.521	55.697	61.438	1.00	38.17	A
	ATOM	723	N	PRO	A	115	64.076	56.435	63.484	1.00	36.13	A
25	ATOM	724	CD	PRO	A	115	65.015	56.886	64.526	1.00	34.15	A
	ATOM	725	CA	PRO	A	115	62.715	56.314	64.011	1.00	34.44	A
	ATOM	726	CB	PRO	A	115	62.815	57.022	65.351	1.00	34.06	A
	ATOM	727	CG	PRO	A	115	64.220	56.680	65.777	1.00	35.33	A
	ATOM	728	C	PRO	A	115	61.694	56.968	63.076	1.00	33.56	A
30	ATOM	729	O	PRO	A	115	60.658	56.384	62.763	1.00	33.50	A
	ATOM	730	N	LEU	A	116	62.001	58.179	62.622	1.00	31.71	A
	ATOM	731	CA	LEU	A	116	61.108	58.903	61.733	1.00	30.40	A
	ATOM	732	CB	LEU	A	116	61.583	60.347	61.567	1.00	29.42	A
	ATOM	733	CG	LEU	A	116	60.603	61.229	60.796	1.00	28.24	A
35	ATOM	734	CD1	LEU	A	116	59.268	61.223	61.507	1.00	28.18	A
	ATOM	735	CD2	LEU	A	116	61.144	62.633	60.674	1.00	29.52	A
	ATOM	736	C	LEU	A	116	61.005	58.211	60.375	1.00	30.54	A
	ATOM	737	O	LEU	A	116	59.909	58.046	59.823	1.00	29.43	A
	ATOM	738	N	LEU	A	117	62.150	57.804	59.836	1.00	30.80	A
40	ATOM	739	CA	LEU	A	117	62.193	57.097	58.555	1.00	30.78	A
	ATOM	740	CB	LEU	A	117	63.632	56.678	58.223	1.00	28.60	A
	ATOM	741	CG	LEU	A	117	63.843	55.833	56.966	1.00	27.90	A
	ATOM	742	CD1	LEU	A	117	63.388	56.587	55.756	1.00	26.40	A
	ATOM	743	CD2	LEU	A	117	65.304	55.467	56.830	1.00	29.33	A
45	ATOM	744	C	LEU	A	117	61.311	55.856	58.624	1.00	32.57	A
	ATOM	745	O	LEU	A	117	60.403	55.675	57.800	1.00	33.66	A
	ATOM	746	N	ASP	A	118	61.588	55.002	59.608	1.00	32.30	A
	ATOM	747	CA	ASP	A	118	60.821	53.781	59.777	1.00	32.82	A
	ATOM	748	CB	ASP	A	118	61.241	53.035	61.046	1.00	34.51	A
50	ATOM	749	CG	ASP	A	118	62.660	52.481	60.958	1.00	38.01	A
	ATOM	750	OD1	ASP	A	118	63.075	52.088	59.841	1.00	37.92	A
	ATOM	751	OD2	ASP	A	118	63.355	52.432	62.007	1.00	38.31	A
	ATOM	752	C	ASP	A	118	59.345	54.104	59.836	1.00	32.67	A
	ATOM	753	O	ASP	A	118	58.533	53.458	59.160	1.00	33.71	A

	ATOM	754	N	ALA	A	119	58.997	55.109	60.632	1.00	31.48	A
	ATOM	755	CA	ALA	A	119	57.600	55.512	60.774	1.00	32.03	A
	ATOM	756	CB	ALA	A	119	57.512	56.753	61.625	1.00	31.77	A
	ATOM	757	C	ALA	A	119	56.961	55.774	59.418	1.00	32.00	A
5	ATOM	758	O	ALA	A	119	55.932	55.185	59.071	1.00	31.09	A
	ATOM	759	N	GLY	A	120	57.582	56.673	58.660	1.00	32.93	A
	ATOM	760	CA	GLY	A	120	57.081	57.007	57.341	1.00	33.63	A
	ATOM	761	C	GLY	A	120	57.019	55.773	56.469	1.00	33.78	A
	ATOM	762	O	GLY	A	120	56.045	55.571	55.748	1.00	33.76	A
10	ATOM	763	N	CYS	A	121	58.056	54.944	56.522	1.00	34.09	A
	ATOM	764	CA	CYS	A	121	58.048	53.735	55.714	1.00	37.06	A
	ATOM	765	CB	CYS	A	121	59.370	52.985	55.852	1.00	37.59	A
	ATOM	766	SG	CYS	A	121	60.672	53.684	54.825	1.00	37.93	A
	ATOM	767	C	CYS	A	121	56.882	52.814	56.063	1.00	36.49	A
15	ATOM	768	O	CYS	A	121	56.222	52.272	55.177	1.00	37.36	A
	ATOM	769	N	LYS	A	122	56.617	52.645	57.348	1.00	36.54	A
	ATOM	770	CA	LYS	A	122	55.525	51.786	57.766	1.00	37.44	A
	ATOM	771	CB	LYS	A	122	55.445	51.751	59.288	1.00	38.22	A
	ATOM	772	CG	LYS	A	122	56.652	51.150	59.950	1.00	38.67	A
20	ATOM	773	CD	LYS	A	122	56.424	51.081	61.441	1.00	42.04	A
	ATOM	774	CE	LYS	A	122	57.663	50.592	62.185	1.00	42.25	A
	ATOM	775	NZ	LYS	A	122	57.394	50.419	63.636	1.00	41.74	A
	ATOM	776	C	LYS	A	122	54.197	52.276	57.208	1.00	36.82	A
	ATOM	777	O	LYS	A	122	53.340	51.479	56.812	1.00	36.50	A
25	ATOM	778	N	VAL	A	123	54.035	53.595	57.187	1.00	36.30	A
	ATOM	779	CA	VAL	A	123	52.810	54.208	56.699	1.00	35.72	A
	ATOM	780	CB	VAL	A	123	52.832	55.718	56.967	1.00	36.26	A
	ATOM	781	CG1	VAL	A	123	51.483	56.319	56.621	1.00	36.90	A
	ATOM	782	CG2	VAL	A	123	53.170	55.966	58.429	1.00	35.63	A
30	ATOM	783	C	VAL	A	123	52.576	53.929	55.208	1.00	35.46	A
	ATOM	784	O	VAL	A	123	51.448	53.633	54.793	1.00	33.96	A
	ATOM	785	N	VAL	A	124	53.639	54.007	54.406	1.00	35.31	A
	ATOM	786	CA	VAL	A	124	53.510	53.737	52.970	1.00	34.89	A
	ATOM	787	CB	VAL	A	124	54.815	54.026	52.177	1.00	34.43	A
35	ATOM	788	CG1	VAL	A	124	54.564	53.832	50.682	1.00	32.55	A
	ATOM	789	CG2	VAL	A	124	55.294	55.442	52.449	1.00	34.56	A
	ATOM	790	C	VAL	A	124	53.135	52.273	52.767	1.00	34.07	A
	ATOM	791	O	VAL	A	124	52.317	51.947	51.898	1.00	34.52	A
	ATOM	792	N	ALA	A	125	53.734	51.401	53.575	1.00	32.52	A
40	ATOM	793	CA	ALA	A	125	53.452	49.974	53.500	1.00	33.46	A
	ATOM	794	CB	ALA	A	125	54.294	49.221	54.496	1.00	31.49	A
	ATOM	795	C	ALA	A	125	51.975	49.757	53.805	1.00	35.59	A
	ATOM	796	O	ALA	A	125	51.283	48.987	53.127	1.00	35.62	A
	ATOM	797	N	GLU	A	126	51.495	50.462	54.823	1.00	37.35	A
45	ATOM	798	CA	GLU	A	126	50.107	50.357	55.213	1.00	37.88	A
	ATOM	799	CB	GLU	A	126	49.864	51.130	56.494	1.00	39.94	A
	ATOM	800	CG	GLU	A	126	50.589	50.522	57.658	1.00	44.44	A
	ATOM	801	CD	GLU	A	126	49.884	50.789	58.974	1.00	47.25	A
	ATOM	802	OE1	GLU	A	126	49.926	51.949	59.454	1.00	46.76	A
50	ATOM	803	OE2	GLU	A	126	49.271	49.832	59.516	1.00	49.61	A
	ATOM	804	C	GLU	A	126	49.149	50.812	54.142	1.00	37.12	A
	ATOM	805	O	GLU	A	126	47.974	50.472	54.189	1.00	36.85	A
	ATOM	806	N	MSE	A	127	49.648	51.573	53.176	1.00	37.83	A
	ATOM	807	CA	MSE	A	127	48.814	52.035	52.085	1.00	38.50	A

5	ATOM	808	CB	MSE	A	127	49.473	53.225	51.396	1.00	39.64	A
	ATOM	809	CG	MSE	A	127	49.682	54.471	52.264	1.00	40.86	A
	ATOM	810	SE	MSE	A	127	50.428	55.994	51.160	1.00	44.01	A
	ATOM	811	CE	MSE	A	127	48.774	56.477	50.261	1.00	43.47	A
	ATOM	812	C	MSE	A	127	48.621	50.885	51.092	1.00	38.76	A
10	ATOM	813	O	MSE	A	127	47.586	50.792	50.443	1.00	38.95	A
	ATOM	814	N	ILE	A	128	49.607	49.997	51.003	1.00	39.74	A
	ATOM	815	CA	ILE	A	128	49.552	48.849	50.090	1.00	40.70	A
	ATOM	816	CB	ILE	A	128	50.989	48.359	49.755	1.00	39.21	A
	ATOM	817	CG2	ILE	A	128	50.935	47.158	48.828	1.00	39.17	A
15	ATOM	818	CG1	ILE	A	128	51.797	49.518	49.163	1.00	37.59	A
	ATOM	819	CD1	ILE	A	128	53.148	49.159	48.595	1.00	35.03	A
	ATOM	820	C	ILE	A	128	48.777	47.698	50.736	1.00	42.24	A
	ATOM	821	O	ILE	A	128	47.886	47.098	50.132	1.00	40.92	A
	ATOM	822	N	ARG	A	129	49.147	47.412	51.980	1.00	46.16	A
20	ATOM	823	CA	ARG	A	129	48.556	46.350	52.792	1.00	49.18	A
	ATOM	824	CB	ARG	A	129	48.696	46.701	54.268	1.00	50.29	A
	ATOM	825	CG	ARG	A	129	48.224	45.614	55.205	1.00	53.92	A
	ATOM	826	CD	ARG	A	129	48.566	45.978	56.643	1.00	58.68	A
	ATOM	827	NE	ARG	A	129	49.936	46.490	56.743	1.00	62.87	A
25	ATOM	828	CZ	ARG	A	129	50.553	46.798	57.881	1.00	64.32	A
	ATOM	829	NH1	ARG	A	129	49.927	46.647	59.045	1.00	64.82	A
	ATOM	830	NH2	ARG	A	129	51.799	47.258	57.850	1.00	64.62	A
	ATOM	831	C	ARG	A	129	47.094	46.044	52.498	1.00	49.27	A
	ATOM	832	O	ARG	A	129	46.230	46.920	52.589	1.00	49.24	A
30	ATOM	833	N	GLY	A	130	46.839	44.785	52.158	1.00	48.73	A
	ATOM	834	CA	GLY	A	130	45.492	44.354	51.873	1.00	49.33	A
	ATOM	835	C	GLY	A	130	44.843	44.937	50.632	1.00	50.07	A
	ATOM	836	O	GLY	A	130	43.619	44.856	50.486	1.00	49.22	A
	ATOM	837	N	ARG	A	131	45.630	45.523	49.735	1.00	49.98	A
35	ATOM	838	CA	ARG	A	131	45.048	46.086	48.524	1.00	50.73	A
	ATOM	839	CB	ARG	A	131	45.402	47.573	48.410	1.00	51.87	A
	ATOM	840	CG	ARG	A	131	44.801	48.429	49.545	1.00	54.75	A
	ATOM	841	CD	ARG	A	131	45.035	49.929	49.340	1.00	57.52	A
	ATOM	842	NE	ARG	A	131	44.412	50.438	48.116	1.00	60.43	A
40	ATOM	843	CZ	ARG	A	131	43.098	50.531	47.910	1.00	61.10	A
	ATOM	844	NH1	ARG	A	131	42.248	50.147	48.855	1.00	60.79	A
	ATOM	845	NH2	ARG	A	131	42.634	51.009	46.755	1.00	61.77	A
	ATOM	846	C	ARG	A	131	45.447	45.325	47.261	1.00	50.69	A
	ATOM	847	O	ARG	A	131	46.432	44.592	47.249	1.00	51.15	A
45	ATOM	848	N	SER	A	132	44.670	45.494	46.199	1.00	50.35	A
	ATOM	849	CA	SER	A	132	44.941	44.798	44.950	1.00	50.32	A
	ATOM	850	CB	SER	A	132	43.630	44.489	44.224	1.00	49.61	A
	ATOM	851	OG	SER	A	132	43.082	45.662	43.648	1.00	48.59	A
	ATOM	852	C	SER	A	132	45.837	45.608	44.023	1.00	50.87	A
50	ATOM	853	O	SER	A	132	46.056	46.808	44.235	1.00	50.23	A
	ATOM	854	N	PRO	A	133	46.359	44.957	42.970	1.00	50.57	A
	ATOM	855	CD	PRO	A	133	46.253	43.520	42.659	1.00	49.65	A
	ATOM	856	CA	PRO	A	133	47.230	45.628	42.006	1.00	50.93	A
	ATOM	857	CB	PRO	A	133	47.392	44.581	40.914	1.00	50.37	A
	ATOM	858	CG	PRO	A	133	47.405	43.315	41.698	1.00	50.36	A
	ATOM	859	C	PRO	A	133	46.616	46.915	41.483	1.00	51.56	A
	ATOM	860	O	PRO	A	133	47.263	47.964	41.480	1.00	52.20	A
	ATOM	861	N	GLU	A	134	45.364	46.839	41.044	1.00	51.94	A

	ATOM	862	CA	GLU	A	134	44.693	48.021	40.516	1.00	52.22	A
	ATOM	863	CB	GLU	A	134	43.395	47.637	39.811	1.00	54.08	A
	ATOM	864	CG	GLU	A	134	43.436	47.886	38.314	1.00	58.97	A
	ATOM	865	CD	GLU	A	134	43.821	49.320	37.974	1.00	62.39	A
5	ATOM	866	OE1	GLU	A	134	43.122	50.254	38.436	1.00	63.15	A
	ATOM	867	OE2	GLU	A	134	44.823	49.513	37.243	1.00	64.67	A
	ATOM	868	C	GLU	A	134	44.406	49.035	41.610	1.00	50.15	A
	ATOM	869	O	GLU	A	134	44.400	50.244	41.355	1.00	49.58	A
	ATOM	870	N	GLU	A	135	44.177	48.539	42.823	1.00	47.26	A
10	ATOM	871	CA	GLU	A	135	43.904	49.412	43.948	1.00	45.19	A
	ATOM	872	CB	GLU	A	135	43.390	48.613	45.142	1.00	44.69	A
	ATOM	873	CG	GLU	A	135	41.973	48.135	44.948	1.00	47.13	A
	ATOM	874	CD	GLU	A	135	41.333	47.585	46.207	1.00	49.00	A
	ATOM	875	OE1	GLU	A	135	41.857	46.590	46.766	1.00	49.49	A
15	ATOM	876	OE2	GLU	A	135	40.295	48.153	46.633	1.00	50.00	A
	ATOM	877	C	GLU	A	135	45.160	50.162	44.328	1.00	43.66	A
	ATOM	878	O	GLU	A	135	45.113	51.349	44.650	1.00	42.57	A
	ATOM	879	N	ILE	A	136	46.288	49.467	44.269	1.00	41.78	A
	ATOM	880	CA	ILE	A	136	47.558	50.077	44.622	1.00	41.23	A
20	ATOM	881	CB	ILE	A	136	48.646	49.014	44.782	1.00	39.22	A
	ATOM	882	CG2	ILE	A	136	49.957	49.675	45.197	1.00	37.75	A
	ATOM	883	CG1	ILE	A	136	48.180	47.970	45.801	1.00	37.01	A
	ATOM	884	CD1	ILE	A	136	49.154	46.847	46.033	1.00	34.37	A
	ATOM	885	C	ILE	A	136	47.993	51.065	43.558	1.00	42.50	A
25	ATOM	886	O	ILE	A	136	48.490	52.162	43.856	1.00	42.93	A
	ATOM	887	N	ARG	A	137	47.787	50.651	42.314	1.00	42.34	A
	ATOM	888	CA	ARG	A	137	48.144	51.439	41.151	1.00	41.82	A
	ATOM	889	CB	ARG	A	137	47.844	50.636	39.884	1.00	42.65	A
	ATOM	890	CG	ARG	A	137	48.949	50.635	38.849	1.00	43.90	A
30	ATOM	891	CD	ARG	A	137	48.594	49.715	37.679	1.00	45.63	A
	ATOM	892	NE	ARG	A	137	48.503	48.315	38.092	1.00	47.76	A
	ATOM	893	CZ	ARG	A	137	47.567	47.477	37.664	1.00	48.21	A
	ATOM	894	NH1	ARG	A	137	46.644	47.901	36.810	1.00	49.10	A
	ATOM	895	NH2	ARG	A	137	47.546	46.226	38.099	1.00	48.10	A
35	ATOM	896	C	ARG	A	137	47.348	52.736	41.156	1.00	40.67	A
	ATOM	897	O	ARG	A	137	47.821	53.773	40.685	1.00	39.93	A
	ATOM	898	N	ARG	A	138	46.134	52.677	41.694	1.00	40.67	A
	ATOM	899	CA	ARG	A	138	45.276	53.864	41.756	1.00	40.88	A
	ATOM	900	CB	ARG	A	138	43.807	53.456	41.932	1.00	39.95	A
40	ATOM	901	CG	ARG	A	138	43.140	52.934	40.660	0.00	41.86	A
	ATOM	902	CD	ARG	A	138	43.070	53.989	39.550	0.00	42.76	A
	ATOM	903	NE	ARG	A	138	44.301	54.072	38.764	0.00	43.72	A
	ATOM	904	CZ	ARG	A	138	44.443	54.802	37.659	0.00	44.10	A
	ATOM	905	NH1	ARG	A	138	43.430	55.523	37.196	0.00	44.35	A
45	ATOM	906	NH2	ARG	A	138	45.602	54.812	37.015	0.00	44.35	A
	ATOM	907	C	ARG	A	138	45.706	54.791	42.895	1.00	39.80	A
	ATOM	908	O	ARG	A	138	45.705	56.016	42.762	1.00	39.09	A
	ATOM	909	N	THR	A	139	46.083	54.177	44.008	1.00	39.87	A
	ATOM	910	CA	THR	A	139	46.544	54.877	45.193	1.00	39.93	A
50	ATOM	911	CB	THR	A	139	47.058	53.872	46.234	1.00	40.30	A
	ATOM	912	OG1	THR	A	139	45.971	53.054	46.689	1.00	40.58	A
	ATOM	913	CG2	THR	A	139	47.684	54.602	47.420	1.00	41.79	A
	ATOM	914	C	THR	A	139	47.674	55.849	44.881	1.00	41.13	A
	ATOM	915	O	THR	A	139	47.752	56.941	45.455	1.00	42.14	A

	ATOM	916	N	PHE	A	140	48.559	55.443	43.978	1.00	41.08	A
	ATOM	917	CA	PHE	A	140	49.705	56.267	43.607	1.00	39.57	A
	ATOM	918	CB	PHE	A	140	50.986	55.449	43.755	1.00	38.91	A
	ATOM	919	CG	PHE	A	140	51.220	54.943	45.145	1.00	38.38	A
5	ATOM	920	CD1	PHE	A	140	51.519	55.824	46.174	1.00	38.13	A
	ATOM	921	CD2	PHE	A	140	51.122	53.588	45.432	1.00	37.94	A
	ATOM	922	CE1	PHE	A	140	51.722	55.364	47.464	1.00	38.18	A
	ATOM	923	CE2	PHE	A	140	51.323	53.118	46.721	1.00	37.42	A
	ATOM	924	CZ	PHE	A	140	51.622	54.008	47.739	1.00	38.51	A
10	ATOM	925	C	PHE	A	140	49.600	56.779	42.185	1.00	39.01	A
	ATOM	926	O	PHE	A	140	50.512	57.434	41.685	1.00	39.06	A
	ATOM	927	N	ASN	A	141	48.485	56.483	41.537	1.00	38.54	A
	ATOM	928	CA	ASN	A	141	48.294	56.894	40.162	1.00	38.58	A
	ATOM	929	CB	ASN	A	141	48.220	58.407	40.049	1.00	39.46	A
15	ATOM	930	CG	ASN	A	141	47.787	58.847	38.669	1.00	41.82	A
	ATOM	931	OD1	ASN	A	141	46.655	58.592	38.257	1.00	44.53	A
	ATOM	932	ND2	ASN	A	141	48.687	59.495	37.938	1.00	42.34	A
	ATOM	933	C	ASN	A	141	49.439	56.378	39.296	1.00	38.74	A
	ATOM	934	O	ASN	A	141	50.031	57.122	38.503	1.00	38.59	A
20	ATOM	935	N	ILE	A	142	49.738	55.093	39.459	1.00	38.05	A
	ATOM	936	CA	ILE	A	142	50.800	54.429	38.715	1.00	37.68	A
	ATOM	937	CB	ILE	A	142	51.425	53.321	39.561	1.00	36.00	A
	ATOM	938	CG2	ILE	A	142	52.451	52.563	38.755	1.00	34.95	A
	ATOM	939	CG1	ILE	A	142	52.021	53.921	40.829	1.00	35.82	A
25	ATOM	940	CD1	ILE	A	142	52.449	52.875	41.837	1.00	36.82	A
	ATOM	941	C	ILE	A	142	50.239	53.819	37.440	1.00	38.81	A
	ATOM	942	O	ILE	A	142	49.121	53.321	37.441	1.00	39.45	A
	ATOM	943	N	VAL	A	143	51.022	53.855	36.361	1.00	40.31	A
	ATOM	944	CA	VAL	A	143	50.620	53.310	35.053	1.00	40.27	A
30	ATOM	945	CB	VAL	A	143	51.373	54.017	33.905	1.00	42.11	A
	ATOM	946	CG1	VAL	A	143	51.035	53.348	32.567	1.00	42.72	A
	ATOM	947	CG2	VAL	A	143	51.016	55.493	33.877	1.00	41.43	A
	ATOM	948	C	VAL	A	143	50.868	51.808	34.881	1.00	39.19	A
	ATOM	949	O	VAL	A	143	51.955	51.309	35.172	1.00	38.15	A
35	ATOM	950	N	ASN	A	144	49.869	51.107	34.359	1.00	38.94	A
	ATOM	951	CA	ASN	A	144	49.968	49.670	34.137	1.00	39.16	A
	ATOM	952	CB	ASN	A	144	48.575	49.048	34.256	1.00	39.51	A
	ATOM	953	CG	ASN	A	144	48.570	47.573	33.959	1.00	40.78	A
	ATOM	954	OD1	ASN	A	144	49.586	46.903	34.090	1.00	44.00	A
40	ATOM	955	ND2	ASN	A	144	47.421	47.052	33.574	1.00	41.05	A
	ATOM	956	C	ASN	A	144	50.582	49.341	32.775	1.00	38.55	A
	ATOM	957	O	ASN	A	144	49.876	48.975	31.839	1.00	37.91	A
	ATOM	958	N	ASP	A	145	51.902	49.448	32.685	1.00	38.25	A
	ATOM	959	CA	ASP	A	145	52.624	49.190	31.440	1.00	39.85	A
45	ATOM	960	CB	ASP	A	145	53.996	49.862	31.498	1.00	39.46	A
	ATOM	961	CG	ASP	A	145	54.766	49.490	32.750	1.00	39.69	A
	ATOM	962	OD1	ASP	A	145	54.213	48.735	33.587	1.00	39.21	A
	ATOM	963	OD2	ASP	A	145	55.918	49.947	32.895	1.00	38.21	A
	ATOM	964	C	ASP	A	145	52.798	47.712	31.092	1.00	40.13	A
50	ATOM	965	O	ASP	A	145	53.702	47.343	30.337	1.00	39.56	A
	ATOM	966	N	PHE	A	146	51.938	46.870	31.652	1.00	40.47	A
	ATOM	967	CA	PHE	A	146	51.978	45.440	31.377	1.00	40.10	A
	ATOM	968	CB	PHE	A	146	51.371	44.644	32.541	1.00	39.31	A
	ATOM	969	CG	PHE	A	146	52.301	44.453	33.699	1.00	40.02	A

	ATOM	970	CD1	PHE	A	146	53.534	43.850	33.520	1.00	39.21	A
	ATOM	971	CD2	PHE	A	146	51.952	44.889	34.971	1.00	39.97	A
	ATOM	972	CE1	PHE	A	146	54.407	43.690	34.591	1.00	39.41	A
	ATOM	973	CE2	PHE	A	146	52.827	44.731	36.051	1.00	38.93	A
5	ATOM	974	CZ	PHE	A	146	54.053	44.131	35.858	1.00	38.17	A
	ATOM	975	C	PHE	A	146	51.167	45.171	30.113	1.00	40.82	A
	ATOM	976	O	PHE	A	146	50.013	45.603	29.999	1.00	41.89	A
	ATOM	977	N	THR	A	147	51.773	44.476	29.154	1.00	40.38	A
	ATOM	978	CA	THR	A	147	51.073	44.137	27.922	1.00	38.81	A
10	ATOM	979	CB	THR	A	147	51.999	43.509	26.877	1.00	38.98	A
	ATOM	980	OG1	THR	A	147	52.651	42.373	27.456	1.00	39.24	A
	ATOM	981	CG2	THR	A	147	53.030	44.498	26.395	1.00	36.50	A
	ATOM	982	C	THR	A	147	50.062	43.070	28.286	1.00	38.78	A
	ATOM	983	O	THR	A	147	50.233	42.343	29.268	1.00	37.08	A
15	ATOM	984	N	PRO	A	148	49.003	42.943	27.485	1.00	39.53	A
	ATOM	985	CD	PRO	A	148	48.718	43.722	26.266	1.00	39.08	A
	ATOM	986	CA	PRO	A	148	47.958	41.947	27.732	1.00	40.59	A
	ATOM	987	CB	PRO	A	148	47.166	41.970	26.428	1.00	39.52	A
	ATOM	988	CG	PRO	A	148	47.260	43.419	26.034	1.00	39.40	A
20	ATOM	989	C	PRO	A	148	48.505	40.545	28.078	1.00	42.69	A
	ATOM	990	O	PRO	A	148	48.007	39.876	28.984	1.00	43.05	A
	ATOM	991	N	GLU	A	149	49.546	40.123	27.370	1.00	45.32	A
	ATOM	992	CA	GLU	A	149	50.155	38.814	27.572	1.00	46.47	A
	ATOM	993	CB	GLU	A	149	51.059	38.496	26.395	1.00	44.18	A
25	ATOM	994	CG	GLU	A	149	51.681	37.137	26.430	1.00	43.56	A
	ATOM	995	CD	GLU	A	149	52.660	36.955	25.311	1.00	43.86	A
	ATOM	996	OE1	GLU	A	149	53.660	37.699	25.279	1.00	43.12	A
	ATOM	997	OE2	GLU	A	149	52.430	36.075	24.458	1.00	44.44	A
	ATOM	998	C	GLU	A	149	50.974	38.773	28.845	1.00	48.79	A
30	ATOM	999	O	GLU	A	149	50.852	37.856	29.660	1.00	49.11	A
	ATOM	1000	N	GLU	A	150	51.826	39.773	29.006	1.00	52.88	A
	ATOM	1001	CA	GLU	A	150	52.676	39.855	30.180	1.00	56.79	A
	ATOM	1002	CB	GLU	A	150	53.548	41.105	30.090	1.00	56.56	A
	ATOM	1003	CG	GLU	A	150	54.707	41.109	31.045	1.00	57.96	A
35	ATOM	1004	CD	GLU	A	150	55.774	40.103	30.660	1.00	59.33	A
	ATOM	1005	OE1	GLU	A	150	55.489	38.887	30.639	1.00	60.34	A
	ATOM	1006	OE2	GLU	A	150	56.907	40.533	30.372	1.00	60.87	A
	ATOM	1007	C	GLU	A	150	51.804	39.913	31.433	1.00	59.23	A
	ATOM	1008	O	GLU	A	150	52.187	39.417	32.488	1.00	59.36	A
40	ATOM	1009	N	GLU	A	151	50.627	40.519	31.305	1.00	62.33	A
	ATOM	1010	CA	GLU	A	151	49.701	40.651	32.424	1.00	64.96	A
	ATOM	1011	CB	GLU	A	151	48.477	41.452	31.982	1.00	65.44	A
	ATOM	1012	CG	GLU	A	151	48.102	42.579	32.923	1.00	66.38	A
	ATOM	1013	CD	GLU	A	151	47.141	43.563	32.287	1.00	67.52	A
45	ATOM	1014	OE1	GLU	A	151	47.510	44.187	31.269	1.00	67.49	A
	ATOM	1015	OE2	GLU	A	151	46.014	43.713	32.803	1.00	68.18	A
	ATOM	1016	C	GLU	A	151	49.270	39.286	32.954	1.00	66.62	A
	ATOM	1017	O	GLU	A	151	49.543	38.943	34.104	1.00	66.87	A
	ATOM	1018	N	ALA	A	152	48.602	38.512	32.106	1.00	68.29	A
50	ATOM	1019	CA	ALA	A	152	48.137	37.181	32.474	1.00	70.15	A
	ATOM	1020	CB	ALA	A	152	47.511	36.503	31.268	1.00	70.09	A
	ATOM	1021	C	ALA	A	152	49.280	36.327	33.014	1.00	71.79	A
	ATOM	1022	O	ALA	A	152	49.085	35.503	33.903	1.00	71.18	A
	ATOM	1023	N	ALA	A	153	50.477	36.526	32.475	1.00	74.38	A

	ATOM	1024	CA	ALA	A	153	51.632	35.761	32.917	1.00	76.96	A
	ATOM	1025	CB	ALA	A	153	52.834	36.056	32.020	1.00	76.52	A
	ATOM	1026	C	ALA	A	153	51.969	36.069	34.376	1.00	79.23	A
	ATOM	1027	O	ALA	A	153	53.040	35.700	34.863	1.00	80.18	A
5	ATOM	1028	N	ILE	A	154	51.061	36.759	35.067	1.00	80.86	A
	ATOM	1029	CA	ILE	A	154	51.257	37.103	36.479	1.00	82.60	A
	ATOM	1030	CB	ILE	A	154	51.680	38.592	36.656	1.00	81.99	A
	ATOM	1031	CG2	ILE	A	154	51.889	38.898	38.134	0.00	82.34	A
	ATOM	1032	CG1	ILE	A	154	52.986	38.866	35.905	1.00	81.41	A
10	ATOM	1033	CD1	ILE	A	154	53.347	40.336	35.822	0.00	81.80	A
	ATOM	1034	C	ILE	A	154	49.976	36.834	37.285	1.00	83.80	A
	ATOM	1035	O	ILE	A	154	49.036	37.633	37.272	1.00	83.56	A
	ATOM	1036	N	ARG	A	155	49.956	35.697	37.982	1.00	85.60	A
	ATOM	1037	CA	ARG	A	155	48.807	35.284	38.783	1.00	86.76	A
15	ATOM	1038	CB	ARG	A	155	48.632	36.208	39.992	0.00	87.40	A
	ATOM	1039	CG	ARG	A	155	49.431	35.788	41.222	0.00	88.39	A
	ATOM	1040	CD	ARG	A	155	50.925	35.725	40.946	0.00	89.22	A
	ATOM	1041	NE	ARG	A	155	51.668	35.196	42.087	0.00	89.99	A
	ATOM	1042	CZ	ARG	A	155	51.561	33.949	42.535	0.00	90.38	A
20	ATOM	1043	NH1	ARG	A	155	50.740	33.095	41.937	0.00	90.63	A
	ATOM	1044	NH2	ARG	A	155	52.272	33.555	43.584	0.00	90.63	A
	ATOM	1045	C	ARG	A	155	47.543	35.286	37.933	1.00	87.04	A
	ATOM	1046	O	ARG	A	155	46.710	36.199	38.125	1.00	87.33	A
	ATOM	1047	OXT	ARG	A	155	47.413	34.380	37.075	1.00	86.76	A
25	ATOM	1048	CB	LEU	B	270	49.350	65.486	42.241	1.00	56.04	B
	ATOM	1049	CG	LEU	B	270	48.859	64.640	41.059	1.00	56.55	B
	ATOM	1050	CD1	LEU	B	270	47.337	64.629	41.020	1.00	55.59	B
	ATOM	1051	CD2	LEU	B	270	49.424	65.209	39.762	1.00	56.75	B
	ATOM	1052	C	LEU	B	270	49.537	63.882	44.208	1.00	54.79	B
30	ATOM	1053	O	LEU	B	270	50.136	63.918	45.287	1.00	55.23	B
	ATOM	1054	N	LEU	B	270	49.056	66.304	44.560	1.00	56.05	B
	ATOM	1055	CA	LEU	B	270	48.835	65.142	43.652	1.00	55.53	B
	ATOM	1056	N	LYS	B	271	49.463	62.779	43.462	1.00	52.96	B
	ATOM	1057	CA	LYS	B	271	50.053	61.495	43.865	1.00	49.38	B
35	ATOM	1058	CB	LYS	B	271	49.292	60.338	43.210	1.00	48.76	B
	ATOM	1059	CG	LYS	B	271	47.793	60.523	43.065	1.00	48.20	B
	ATOM	1060	CD	LYS	B	271	47.049	59.967	44.264	1.00	48.26	B
	ATOM	1061	CE	LYS	B	271	45.545	59.892	44.014	1.00	46.84	B
	ATOM	1062	NZ	LYS	B	271	45.188	59.152	42.766	1.00	47.61	B
40	ATOM	1063	C	LYS	B	271	51.521	61.364	43.462	1.00	47.55	B
	ATOM	1064	O	LYS	B	271	52.069	62.218	42.764	1.00	47.27	B
	ATOM	1065	N	ARG	B	272	52.138	60.263	43.883	1.00	45.44	B
	ATOM	1066	CA	ARG	B	272	53.529	59.981	43.558	1.00	42.97	B
	ATOM	1067	CB	ARG	B	272	54.444	60.845	44.404	1.00	42.52	B
45	ATOM	1068	CG	ARG	B	272	55.897	60.542	44.181	1.00	44.05	B
	ATOM	1069	CD	ARG	B	272	56.741	61.677	44.691	1.00	45.19	B
	ATOM	1070	NE	ARG	B	272	57.927	61.836	43.866	1.00	46.68	B
	ATOM	1071	CZ	ARG	B	272	58.416	63.009	43.491	1.00	47.36	B
	ATOM	1072	NH1	ARG	B	272	57.816	64.130	43.868	1.00	46.52	B
50	ATOM	1073	NH2	ARG	B	272	59.505	63.056	42.737	1.00	48.34	B
	ATOM	1074	C	ARG	B	272	53.911	58.517	43.753	1.00	41.43	B
	ATOM	1075	O	ARG	B	272	53.678	57.944	44.816	1.00	41.22	B
	ATOM	1076	N	ASP	B	273	54.495	57.911	42.724	1.00	39.99	B
	ATOM	1077	CA	ASP	B	273	54.914	56.517	42.821	1.00	37.49	B

5	ATOM	1078	CB	ASP	B	273	55.435	56.006	41.487	1.00	38.41	B
	ATOM	1079	CG	ASP	B	273	55.631	54.508	41.482	1.00	40.70	B
	ATOM	1080	OD1	ASP	B	273	56.269	53.969	42.423	1.00	39.39	B
	ATOM	1081	OD2	ASP	B	273	55.143	53.874	40.525	1.00	43.85	B
	ATOM	1082	C	ASP	B	273	56.040	56.474	43.829	1.00	35.40	B
10	ATOM	1083	O	ASP	B	273	57.218	56.453	43.463	1.00	33.99	B
	ATOM	1084	N	LEU	B	274	55.671	56.460	45.101	1.00	33.28	B
	ATOM	1085	CA	LEU	B	274	56.646	56.450	46.170	1.00	32.55	B
	ATOM	1086	CB	LEU	B	274	55.937	56.322	47.514	1.00	32.85	B
	ATOM	1087	CG	LEU	B	274	55.728	57.659	48.229	1.00	34.16	B
15	ATOM	1088	CD1	LEU	B	274	54.930	58.598	47.361	1.00	33.65	B
	ATOM	1089	CD2	LEU	B	274	55.035	57.421	49.561	1.00	35.07	B
	ATOM	1090	C	LEU	B	274	57.723	55.391	46.066	1.00	31.70	B
	ATOM	1091	O	LEU	B	274	58.903	55.687	46.250	1.00	31.68	B
	ATOM	1092	N	ILE	B	275	57.338	54.160	45.756	1.00	31.28	B
20	ATOM	1093	CA	ILE	B	275	58.338	53.115	45.687	1.00	30.61	B
	ATOM	1094	CB	ILE	B	275	57.703	51.700	45.636	1.00	31.77	B
	ATOM	1095	CG2	ILE	B	275	56.364	51.696	46.322	1.00	29.79	B
	ATOM	1096	CG1	ILE	B	275	57.579	51.245	44.196	1.00	34.36	B
	ATOM	1097	CD1	ILE	B	275	58.058	49.838	44.000	1.00	34.82	B
25	ATOM	1098	C	ILE	B	275	59.325	53.301	44.535	1.00	29.10	B
	ATOM	1099	O	ILE	B	275	60.495	52.944	44.675	1.00	28.41	B
	ATOM	1100	N	THR	B	276	58.893	53.846	43.398	1.00	28.07	B
	ATOM	1101	CA	THR	B	276	59.875	54.056	42.336	1.00	29.79	B
	ATOM	1102	CB	THR	B	276	59.259	54.160	40.906	1.00	29.82	B
30	ATOM	1103	OG1	THR	B	276	58.327	55.236	40.859	1.00	33.40	B
	ATOM	1104	CG2	THR	B	276	58.569	52.869	40.507	1.00	31.42	B
	ATOM	1105	C	THR	B	276	60.718	55.314	42.580	1.00	28.87	B
	ATOM	1106	O	THR	B	276	61.885	55.341	42.222	1.00	29.74	B
	ATOM	1107	N	SER	B	277	60.145	56.333	43.211	1.00	27.47	B
35	ATOM	1108	CA	SER	B	277	60.867	57.567	43.454	1.00	27.08	B
	ATOM	1109	CB	SER	B	277	59.877	58.706	43.664	1.00	28.54	B
	ATOM	1110	OG	SER	B	277	59.027	58.861	42.533	1.00	29.07	B
	ATOM	1111	C	SER	B	277	61.843	57.511	44.622	1.00	28.04	B
	ATOM	1112	O	SER	B	277	62.850	58.200	44.607	1.00	29.44	B
40	ATOM	1113	N	LEU	B	278	61.546	56.717	45.644	1.00	28.55	B
	ATOM	1114	CA	LEU	B	278	62.443	56.606	46.786	1.00	28.04	B
	ATOM	1115	CB	LEU	B	278	61.777	55.854	47.921	1.00	27.87	B
	ATOM	1116	CG	LEU	B	278	61.098	56.650	49.043	1.00	29.93	B
	ATOM	1117	CD1	LEU	B	278	62.130	57.593	49.658	1.00	30.19	B
45	ATOM	1118	CD2	LEU	B	278	59.898	57.407	48.526	1.00	28.70	B
	ATOM	1119	C	LEU	B	278	63.697	55.857	46.401	1.00	29.78	B
	ATOM	1120	O	LEU	B	278	63.728	55.140	45.398	1.00	30.41	B
	ATOM	1121	N	PRO	B	279	64.771	56.039	47.171	1.00	30.02	B
	ATOM	1122	CD	PRO	B	279	65.103	57.050	48.187	1.00	29.94	B
50	ATOM	1123	CA	PRO	B	279	65.948	55.281	46.764	1.00	30.32	B
	ATOM	1124	CB	PRO	B	279	67.068	55.907	47.584	1.00	29.20	B
	ATOM	1125	CG	PRO	B	279	66.371	56.499	48.763	1.00	31.41	B
	ATOM	1126	C	PRO	B	279	65.690	53.813	47.094	1.00	32.64	B
	ATOM	1127	O	PRO	B	279	64.946	53.494	48.026	1.00	32.21	B
	ATOM	1128	N	PHE	B	280	66.291	52.927	46.308	1.00	34.93	B
	ATOM	1129	CA	PHE	B	280	66.122	51.495	46.476	1.00	35.83	B
	ATOM	1130	CB	PHE	B	280	67.177	50.745	45.671	1.00	35.18	B
	ATOM	1131	CG	PHE	B	280	67.040	49.266	45.752	1.00	35.73	B

	ATOM	1132	CD1	PHE	B	280	65.871	48.644	45.307	1.00	35.82	B
	ATOM	1133	CD2	PHE	B	280	68.050	48.493	46.319	1.00	34.88	B
	ATOM	1134	CE1	PHE	B	280	65.703	47.266	45.430	1.00	37.94	B
	ATOM	1135	CE2	PHE	B	280	67.897	47.111	46.452	1.00	36.63	B
5	ATOM	1136	CZ	PHE	B	280	66.717	46.489	46.006	1.00	36.74	B
	ATOM	1137	C	PHE	B	280	66.172	51.017	47.917	1.00	37.41	B
	ATOM	1138	O	PHE	B	280	65.263	50.331	48.371	1.00	39.64	B
	ATOM	1139	N	GLU	B	281	67.235	51.366	48.634	1.00	38.02	B
	ATOM	1140	CA	GLU	B	281	67.391	50.934	50.017	1.00	38.96	B
10	ATOM	1141	CB	GLU	B	281	68.622	51.584	50.659	1.00	42.67	B
	ATOM	1142	CG	GLU	B	281	69.932	51.424	49.875	1.00	49.17	B
	ATOM	1143	CD	GLU	B	281	70.188	49.992	49.394	1.00	51.93	B
	ATOM	1144	OE1	GLU	B	281	69.840	49.030	50.127	1.00	51.55	B
	ATOM	1145	OE2	GLU	B	281	70.747	49.845	48.276	1.00	53.97	B
15	ATOM	1146	C	GLU	B	281	66.169	51.251	50.859	1.00	38.70	B
	ATOM	1147	O	GLU	B	281	65.863	50.516	51.796	1.00	40.56	B
	ATOM	1148	N	ILE	B	282	65.472	52.338	50.531	1.00	36.39	B
	ATOM	1149	CA	ILE	B	282	64.289	52.728	51.291	1.00	33.47	B
	ATOM	1150	CB	ILE	B	282	64.019	54.250	51.194	1.00	33.48	B
20	ATOM	1151	CG2	ILE	B	282	62.633	54.581	51.721	1.00	31.07	B
	ATOM	1152	CG1	ILE	B	282	65.091	55.007	51.974	1.00	33.33	B
	ATOM	1153	CD1	ILE	B	282	64.849	56.494	52.090	1.00	35.69	B
	ATOM	1154	C	ILE	B	282	63.030	51.984	50.891	1.00	32.60	B
	ATOM	1155	O	ILE	B	282	62.238	51.614	51.748	1.00	33.74	B
25	ATOM	1156	N	SER	B	283	62.833	51.753	49.602	1.00	32.28	B
	ATOM	1157	CA	SER	B	283	61.632	51.052	49.180	1.00	31.76	B
	ATOM	1158	CB	SER	B	283	61.531	51.043	47.665	1.00	30.24	B
	ATOM	1159	OG	SER	B	283	60.948	52.260	47.227	1.00	30.65	B
	ATOM	1160	C	SER	B	283	61.554	49.642	49.732	1.00	32.64	B
30	ATOM	1161	O	SER	B	283	60.460	49.145	50.033	1.00	31.74	B
	ATOM	1162	N	LEU	B	284	62.715	49.011	49.891	1.00	34.08	B
	ATOM	1163	CA	LEU	B	284	62.761	47.661	50.433	1.00	36.79	B
	ATOM	1164	CB	LEU	B	284	64.158	47.070	50.303	1.00	38.54	B
	ATOM	1165	CG	LEU	B	284	64.620	46.663	48.913	1.00	40.73	B
35	ATOM	1166	CD1	LEU	B	284	65.953	45.935	49.085	1.00	41.39	B
	ATOM	1167	CD2	LEU	B	284	63.598	45.746	48.237	1.00	39.81	B
	ATOM	1168	C	LEU	B	284	62.331	47.606	51.903	1.00	37.57	B
	ATOM	1169	O	LEU	B	284	61.731	46.629	52.333	1.00	37.16	B
	ATOM	1170	N	LYS	B	285	62.654	48.636	52.679	1.00	37.42	B
40	ATOM	1171	CA	LYS	B	285	62.258	48.638	54.071	1.00	37.32	B
	ATOM	1172	CB	LYS	B	285	62.706	49.927	54.757	1.00	37.90	B
	ATOM	1173	CG	LYS	B	285	64.221	50.101	54.711	1.00	41.29	B
	ATOM	1174	CD	LYS	B	285	64.714	51.417	55.305	1.00	43.06	B
	ATOM	1175	CE	LYS	B	285	64.504	51.487	56.811	1.00	44.78	B
45	ATOM	1176	NZ	LYS	B	285	63.347	52.365	57.139	1.00	44.95	B
	ATOM	1177	C	LYS	B	285	60.754	48.531	54.078	1.00	36.58	B
	ATOM	1178	O	LYS	B	285	60.170	47.774	54.859	1.00	36.75	B
	ATOM	1179	N	ILE	B	286	60.137	49.268	53.163	1.00	34.81	B
	ATOM	1180	CA	ILE	B	286	58.687	49.286	53.038	1.00	34.65	B
50	ATOM	1181	CB	ILE	B	286	58.233	50.340	51.988	1.00	35.18	B
	ATOM	1182	CG2	ILE	B	286	56.723	50.435	51.961	1.00	34.75	B
	ATOM	1183	CG1	ILE	B	286	58.778	51.721	52.361	1.00	36.78	B
	ATOM	1184	CD1	ILE	B	286	58.517	52.777	51.304	1.00	35.35	B
	ATOM	1185	C	ILE	B	286	58.141	47.909	52.646	1.00	34.49	B

5	ATOM	1186	O	ILE	B	286	57.109	47.469	53.163	1.00	34.87	B
	ATOM	1187	N	PHE	B	287	58.825	47.232	51.726	1.00	32.88	B
	ATOM	1188	CA	PHE	B	287	58.373	45.915	51.300	1.00	30.31	B
	ATOM	1189	CB	PHE	B	287	59.086	45.501	50.002	1.00	26.38	B
	ATOM	1190	CG	PHE	B	287	58.530	46.184	48.785	1.00	23.19	B
10	ATOM	1191	CD1	PHE	B	287	57.189	46.000	48.444	1.00	21.80	B
	ATOM	1192	CD2	PHE	B	287	59.300	47.078	48.043	1.00	20.28	B
	ATOM	1193	CE1	PHE	B	287	56.617	46.699	47.397	1.00	21.72	B
	ATOM	1194	CE2	PHE	B	287	58.740	47.788	46.985	1.00	21.62	B
	ATOM	1195	CZ	PHE	B	287	57.389	47.599	46.659	1.00	23.65	B
15	ATOM	1196	C	PHE	B	287	58.566	44.899	52.419	1.00	31.61	B
	ATOM	1197	O	PHE	B	287	57.864	43.887	52.487	1.00	32.92	B
	ATOM	1198	N	ASN	B	288	59.498	45.191	53.320	1.00	32.92	B
	ATOM	1199	CA	ASN	B	288	59.747	44.316	54.460	1.00	34.33	B
	ATOM	1200	CB	ASN	B	288	61.117	44.574	55.067	1.00	34.27	B
20	ATOM	1201	CG	ASN	B	288	62.228	43.993	54.243	1.00	35.15	B
	ATOM	1202	OD1	ASN	B	288	62.325	42.768	54.077	1.00	34.77	B
	ATOM	1203	ND2	ASN	B	288	63.086	44.865	53.717	1.00	37.02	B
	ATOM	1204	C	ASN	B	288	58.699	44.515	55.538	1.00	34.60	B
	ATOM	1205	O	ASN	B	288	58.700	43.801	56.537	1.00	35.55	B
25	ATOM	1206	N	TYR	B	289	57.833	45.507	55.347	1.00	33.60	B
	ATOM	1207	CA	TYR	B	289	56.757	45.786	56.286	1.00	32.28	B
	ATOM	1208	CB	TYR	B	289	56.597	47.288	56.536	1.00	30.88	B
	ATOM	1209	CG	TYR	B	289	57.639	47.906	57.444	1.00	31.04	B
	ATOM	1210	CD1	TYR	B	289	57.824	47.445	58.743	1.00	29.76	B
30	ATOM	1211	CE1	TYR	B	289	58.783	48.005	59.577	1.00	28.80	B
	ATOM	1212	CD2	TYR	B	289	58.441	48.954	57.001	1.00	30.42	B
	ATOM	1213	CE2	TYR	B	289	59.404	49.520	57.828	1.00	30.11	B
	ATOM	1214	CZ	TYR	B	289	59.572	49.036	59.117	1.00	29.29	B
	ATOM	1215	OH	TYR	B	289	60.550	49.565	59.927	1.00	27.49	B
35	ATOM	1216	C	TYR	B	289	55.454	45.259	55.712	1.00	33.20	B
	ATOM	1217	O	TYR	B	289	54.381	45.681	56.131	1.00	34.61	B
	ATOM	1218	N	LEU	B	290	55.538	44.348	54.750	1.00	32.98	B
	ATOM	1219	CA	LEU	B	290	54.335	43.794	54.148	1.00	33.98	B
	ATOM	1220	CB	LEU	B	290	54.181	44.325	52.736	1.00	33.99	B
40	ATOM	1221	CG	LEU	B	290	53.894	45.813	52.594	1.00	34.25	B
	ATOM	1222	CD1	LEU	B	290	53.690	46.102	51.123	1.00	32.35	B
	ATOM	1223	CD2	LEU	B	290	52.629	46.192	53.393	1.00	35.31	B
	ATOM	1224	C	LEU	B	290	54.340	42.284	54.112	1.00	35.59	B
	ATOM	1225	O	LEU	B	290	55.366	41.686	53.832	1.00	37.73	B
45	ATOM	1226	N	GLN	B	291	53.200	41.660	54.390	1.00	36.68	B
	ATOM	1227	CA	GLN	B	291	53.126	40.198	54.364	1.00	37.99	B
	ATOM	1228	CB	GLN	B	291	51.808	39.715	54.956	1.00	39.90	B
	ATOM	1229	CG	GLN	B	291	51.514	40.243	56.338	1.00	42.72	B
	ATOM	1230	CD	GLN	B	291	50.510	39.378	57.067	1.00	45.38	B
50	ATOM	1231	OE1	GLN	B	291	49.376	39.196	56.609	1.00	45.17	B
	ATOM	1232	NE2	GLN	B	291	50.925	38.824	58.209	1.00	48.06	B
	ATOM	1233	C	GLN	B	291	53.254	39.696	52.937	1.00	37.97	B
	ATOM	1234	O	GLN	B	291	52.727	40.304	52.005	1.00	37.21	B
	ATOM	1235	N	PHE	B	292	53.924	38.566	52.769	1.00	39.53	B
	ATOM	1236	CA	PHE	B	292	54.154	38.038	51.430	1.00	42.10	B
	ATOM	1237	CB	PHE	B	292	54.592	36.565	51.510	1.00	43.75	B
	ATOM	1238	CG	PHE	B	292	53.463	35.605	51.727	1.00	44.90	B
	ATOM	1239	CD1	PHE	B	292	52.799	35.038	50.641	1.00	43.90	B

	ATOM	1240	CD2	PHE	B	292	53.050	35.280	53.014	1.00	45.10	B
	ATOM	1241	CE1	PHE	B	292	51.742	34.161	50.831	1.00	43.67	B
	ATOM	1242	CE2	PHE	B	292	51.992	34.403	53.217	1.00	44.65	B
	ATOM	1243	CZ	PHE	B	292	51.336	33.842	52.121	1.00	44.41	B
5	ATOM	1244	C	PHE	B	292	52.990	38.217	50.441	1.00	42.01	B
	ATOM	1245	O	PHE	B	292	53.214	38.553	49.280	1.00	43.29	B
	ATOM	1246	N	GLU	B	293	51.753	38.018	50.884	1.00	41.02	B
	ATOM	1247	CA	GLU	B	293	50.605	38.176	49.985	1.00	40.82	B
	ATOM	1248	CB	GLU	B	293	49.289	38.028	50.769	1.00	41.39	B
10	ATOM	1249	CG	GLU	B	293	49.056	36.617	51.350	1.00	42.89	B
	ATOM	1250	CD	GLU	B	293	49.451	36.480	52.818	1.00	43.53	B
	ATOM	1251	OE1	GLU	B	293	50.507	37.006	53.222	1.00	44.09	B
	ATOM	1252	OE2	GLU	B	293	48.704	35.825	53.572	1.00	45.55	B
	ATOM	1253	C	GLU	B	293	50.641	39.524	49.258	1.00	40.05	B
15	ATOM	1254	O	GLU	B	293	50.375	39.603	48.056	1.00	38.85	B
	ATOM	1255	N	ASP	B	294	50.991	40.573	50.000	1.00	40.23	B
	ATOM	1256	CA	ASP	B	294	51.074	41.923	49.450	1.00	40.33	B
	ATOM	1257	CB	ASP	B	294	51.198	42.958	50.579	1.00	41.12	B
	ATOM	1258	CG	ASP	B	294	49.949	43.030	51.464	1.00	42.16	B
20	ATOM	1259	OD1	ASP	B	294	48.815	42.987	50.925	1.00	43.30	B
	ATOM	1260	OD2	ASP	B	294	50.099	43.150	52.699	1.00	41.57	B
	ATOM	1261	C	ASP	B	294	52.259	42.074	48.490	1.00	38.83	B
	ATOM	1262	O	ASP	B	294	52.151	42.714	47.446	1.00	37.73	B
	ATOM	1263	N	ILE	B	295	53.390	41.477	48.840	1.00	37.53	B
25	ATOM	1264	CA	ILE	B	295	54.561	41.573	47.994	1.00	36.43	B
	ATOM	1265	CB	ILE	B	295	55.751	40.853	48.638	1.00	35.75	B
	ATOM	1266	CG2	ILE	B	295	56.926	40.801	47.660	1.00	35.40	B
	ATOM	1267	CG1	ILE	B	295	56.107	41.574	49.950	1.00	36.24	B
	ATOM	1268	CD1	ILE	B	295	57.303	41.033	50.709	1.00	36.08	B
30	ATOM	1269	C	ILE	B	295	54.257	40.987	46.623	1.00	36.37	B
	ATOM	1270	O	ILE	B	295	54.707	41.504	45.593	1.00	36.01	B
	ATOM	1271	N	ILE	B	296	53.470	39.919	46.616	1.00	36.36	B
	ATOM	1272	CA	ILE	B	296	53.094	39.262	45.375	1.00	36.96	B
	ATOM	1273	CB	ILE	B	296	52.329	37.967	45.665	1.00	37.13	B
35	ATOM	1274	CG2	ILE	B	296	51.771	37.366	44.389	1.00	37.11	B
	ATOM	1275	CG1	ILE	B	296	53.276	36.961	46.288	1.00	36.41	B
	ATOM	1276	CD1	ILE	B	296	52.601	35.679	46.620	1.00	38.88	B
	ATOM	1277	C	ILE	B	296	52.256	40.159	44.473	1.00	36.89	B
	ATOM	1278	O	ILE	B	296	52.554	40.297	43.293	1.00	37.07	B
40	ATOM	1279	N	ASN	B	297	51.208	40.769	45.008	1.00	37.95	B
	ATOM	1280	CA	ASN	B	297	50.385	41.649	44.186	1.00	38.86	B
	ATOM	1281	CB	ASN	B	297	49.240	42.246	44.980	1.00	41.69	B
	ATOM	1282	CG	ASN	B	297	48.368	41.213	45.583	1.00	43.05	B
	ATOM	1283	OD1	ASN	B	297	47.914	40.293	44.897	1.00	44.19	B
45	ATOM	1284	ND2	ASN	B	297	48.114	41.345	46.880	1.00	43.88	B
	ATOM	1285	C	ASN	B	297	51.207	42.810	43.705	1.00	37.72	B
	ATOM	1286	O	ASN	B	297	50.953	43.360	42.632	1.00	36.87	B
	ATOM	1287	N	SER	B	298	52.167	43.207	44.531	1.00	36.60	B
	ATOM	1288	CA	SER	B	298	53.006	44.339	44.194	1.00	35.31	B
50	ATOM	1289	CB	SER	B	298	53.926	44.673	45.366	1.00	32.10	B
	ATOM	1290	OG	SER	B	298	53.156	45.195	46.435	1.00	29.27	B
	ATOM	1291	C	SER	B	298	53.784	44.022	42.939	1.00	35.81	B
	ATOM	1292	O	SER	B	298	54.037	44.901	42.111	1.00	35.32	B
	ATOM	1293	N	LEU	B	299	54.136	42.750	42.793	1.00	36.25	B

5	ATOM	1294	CA	LEU	B	299	54.871	42.291	41.625	1.00	36.42	B
	ATOM	1295	CB	LEU	B	299	55.218	40.814	41.771	1.00	35.83	B
	ATOM	1296	CG	LEU	B	299	56.431	40.528	42.654	1.00	36.52	B
	ATOM	1297	CD1	LEU	B	299	56.674	39.028	42.727	1.00	37.64	B
	ATOM	1298	CD2	LEU	B	299	57.655	41.224	42.065	1.00	35.78	B
10	ATOM	1299	C	LEU	B	299	54.082	42.509	40.343	1.00	36.00	B
	ATOM	1300	O	LEU	B	299	54.660	42.539	39.256	1.00	36.92	B
	ATOM	1301	N	GLY	B	300	52.769	42.678	40.474	1.00	35.04	B
	ATOM	1302	CA	GLY	B	300	51.940	42.890	39.303	1.00	35.67	B
	ATOM	1303	C	GLY	B	300	51.417	44.305	39.186	1.00	35.69	B
15	ATOM	1304	O	GLY	B	300	50.538	44.602	38.379	1.00	35.37	B
	ATOM	1305	N	VAL	B	301	51.958	45.194	39.998	1.00	36.32	B
	ATOM	1306	CA	VAL	B	301	51.523	46.569	39.969	1.00	36.62	B
	ATOM	1307	CB	VAL	B	301	51.953	47.291	41.247	1.00	37.56	B
	ATOM	1308	CG1	VAL	B	301	51.752	48.789	41.087	1.00	37.50	B
20	ATOM	1309	CG2	VAL	B	301	51.133	46.752	42.436	1.00	35.20	B
	ATOM	1310	C	VAL	B	301	52.071	47.288	38.751	1.00	36.72	B
	ATOM	1311	O	VAL	B	301	51.321	47.910	38.017	1.00	37.30	B
	ATOM	1312	N	SER	B	302	53.378	47.201	38.534	1.00	37.60	B
	ATOM	1313	CA	SER	B	302	54.005	47.844	37.382	1.00	37.90	B
25	ATOM	1314	CB	SER	B	302	54.317	49.311	37.684	1.00	37.39	B
	ATOM	1315	OG	SER	B	302	55.530	49.417	38.419	1.00	36.20	B
	ATOM	1316	C	SER	B	302	55.316	47.129	37.067	1.00	39.64	B
	ATOM	1317	O	SER	B	302	55.867	46.392	37.901	1.00	38.64	B
	ATOM	1318	N	GLN	B	303	55.821	47.371	35.861	1.00	40.39	B
30	ATOM	1319	CA	GLN	B	303	57.087	46.781	35.428	1.00	41.46	B
	ATOM	1320	CB	GLN	B	303	57.436	47.239	34.013	1.00	41.20	B
	ATOM	1321	CG	GLN	B	303	56.696	46.481	32.950	1.00	43.64	B
	ATOM	1322	CD	GLN	B	303	57.199	45.068	32.815	1.00	44.54	B
	ATOM	1323	OE1	GLN	B	303	57.771	44.517	33.751	1.00	46.50	B
35	ATOM	1324	NE2	GLN	B	303	56.986	44.466	31.650	1.00	44.23	B
	ATOM	1325	C	GLN	B	303	58.241	47.140	36.360	1.00	41.74	B
	ATOM	1326	O	GLN	B	303	59.163	46.345	36.561	1.00	41.80	B
	ATOM	1327	N	ASN	B	304	58.194	48.338	36.928	1.00	42.15	B
	ATOM	1328	CA	ASN	B	304	59.251	48.758	37.826	1.00	41.69	B
40	ATOM	1329	CB	ASN	B	304	59.237	50.263	38.014	1.00	43.58	B
	ATOM	1330	CG	ASN	B	304	60.623	50.861	37.924	1.00	45.74	B
	ATOM	1331	OD1	ASN	B	304	61.599	50.302	38.459	1.00	46.54	B
	ATOM	1332	ND2	ASN	B	304	60.728	52.009	37.240	1.00	47.34	B
	ATOM	1333	C	ASN	B	304	59.130	48.100	39.174	1.00	41.16	B
45	ATOM	1334	O	ASN	B	304	60.126	47.650	39.739	1.00	40.69	B
	ATOM	1335	N	TRP	B	305	57.910	48.060	39.700	1.00	40.22	B
	ATOM	1336	CA	TRP	B	305	57.687	47.439	40.992	1.00	39.44	B
	ATOM	1337	CB	TRP	B	305	56.201	47.464	41.357	1.00	40.05	B
	ATOM	1338	CG	TRP	B	305	55.742	48.762	41.945	1.00	41.46	B
50	ATOM	1339	CD2	TRP	B	305	54.933	48.939	43.120	1.00	42.85	B
	ATOM	1340	CE2	TRP	B	305	54.724	50.324	43.277	1.00	43.18	B
	ATOM	1341	CE3	TRP	B	305	54.363	48.060	44.054	1.00	43.70	B
	ATOM	1342	CD1	TRP	B	305	55.983	50.007	41.456	1.00	41.95	B
	ATOM	1343	NE1	TRP	B	305	55.375	50.953	42.248	1.00	43.45	B
	ATOM	1344	CZ2	TRP	B	305	53.966	50.858	44.336	1.00	43.29	B
	ATOM	1345	CZ3	TRP	B	305	53.608	48.591	45.108	1.00	43.59	B
	ATOM	1346	CH2	TRP	B	305	53.419	49.976	45.237	1.00	43.13	B
	ATOM	1347	C	TRP	B	305	58.186	46.007	40.930	1.00	39.39	B

	ATOM	1348	O	TRP	B	305	58.909	45.556	41.818	1.00	40.05	B
	ATOM	1349	N	ASN	B	306	57.808	45.300	39.868	1.00	38.31	B
	ATOM	1350	CA	ASN	B	306	58.213	43.915	39.699	1.00	36.89	B
	ATOM	1351	CB	ASN	B	306	57.558	43.318	38.449	1.00	39.69	B
5	ATOM	1352	CG	ASN	B	306	57.874	41.836	38.265	1.00	41.87	B
	ATOM	1353	OD1	ASN	B	306	58.898	41.465	37.690	1.00	42.36	B
	ATOM	1354	ND2	ASN	B	306	56.989	40.983	38.763	1.00	44.37	B
	ATOM	1355	C	ASN	B	306	59.730	43.817	39.608	1.00	35.41	B
	ATOM	1356	O	ASN	B	306	60.333	42.902	40.170	1.00	35.33	B
10	ATOM	1357	N	LYS	B	307	60.353	44.765	38.917	1.00	34.02	B
	ATOM	1358	CA	LYS	B	307	61.804	44.750	38.786	1.00	34.18	B
	ATOM	1359	CB	LYS	B	307	62.245	45.720	37.686	1.00	34.16	B
	ATOM	1360	CG	LYS	B	307	63.753	45.889	37.572	1.00	34.46	B
	ATOM	1361	CD	LYS	B	307	64.121	46.934	36.524	1.00	36.66	B
15	ATOM	1362	CE	LYS	B	307	63.783	46.479	35.089	1.00	39.17	B
	ATOM	1363	NZ	LYS	B	307	62.308	46.327	34.816	1.00	41.27	B
	ATOM	1364	C	LYS	B	307	62.491	45.096	40.110	1.00	34.15	B
	ATOM	1365	O	LYS	B	307	63.484	44.476	40.486	1.00	35.79	B
	ATOM	1366	N	ILE	B	308	61.967	46.089	40.814	1.00	33.56	B
20	ATOM	1367	CA	ILE	B	308	62.539	46.483	42.090	1.00	32.11	B
	ATOM	1368	CB	ILE	B	308	61.790	47.706	42.670	1.00	31.25	B
	ATOM	1369	CG2	ILE	B	308	62.235	47.954	44.118	1.00	29.28	B
	ATOM	1370	CG1	ILE	B	308	62.010	48.918	41.746	1.00	30.74	B
	ATOM	1371	CD1	ILE	B	308	61.163	50.148	42.057	1.00	30.81	B
25	ATOM	1372	C	ILE	B	308	62.455	45.330	43.083	1.00	32.53	B
	ATOM	1373	O	ILE	B	308	63.432	44.996	43.741	1.00	33.24	B
	ATOM	1374	N	ILE	B	309	61.288	44.706	43.174	1.00	32.71	B
	ATOM	1375	CA	ILE	B	309	61.094	43.616	44.120	1.00	32.29	B
	ATOM	1376	CB	ILE	B	309	59.605	43.255	44.224	1.00	31.48	B
30	ATOM	1377	CG2	ILE	B	309	59.436	41.944	44.993	1.00	28.42	B
	ATOM	1378	CG1	ILE	B	309	58.860	44.419	44.894	1.00	29.43	B
	ATOM	1379	CD1	ILE	B	309	57.377	44.244	45.030	1.00	29.32	B
	ATOM	1380	C	ILE	B	309	61.881	42.360	43.801	1.00	32.95	B
	ATOM	1381	O	ILE	B	309	62.297	41.616	44.705	1.00	33.10	B
35	ATOM	1382	N	ARG	B	310	62.088	42.120	42.515	1.00	32.48	B
	ATOM	1383	CA	ARG	B	310	62.807	40.929	42.113	1.00	31.41	B
	ATOM	1384	CB	ARG	B	310	62.401	40.562	40.701	1.00	30.53	B
	ATOM	1385	CG	ARG	B	310	61.047	39.954	40.749	1.00	32.30	B
	ATOM	1386	CD	ARG	B	310	60.974	38.823	39.812	1.00	33.94	B
40	ATOM	1387	NE	ARG	B	310	60.659	39.310	38.485	1.00	36.53	B
	ATOM	1388	CZ	ARG	B	310	60.989	38.682	37.369	1.00	37.75	B
	ATOM	1389	NH1	ARG	B	310	61.656	37.535	37.428	1.00	36.97	B
	ATOM	1390	NH2	ARG	B	310	60.649	39.205	36.200	1.00	38.45	B
	ATOM	1391	C	ARG	B	310	64.302	41.065	42.259	1.00	30.16	B
45	ATOM	1392	O	ARG	B	310	65.059	40.091	42.152	1.00	28.61	B
	ATOM	1393	N	LYS	B	311	64.717	42.283	42.552	1.00	29.95	B
	ATOM	1394	CA	LYS	B	311	66.122	42.542	42.727	1.00	31.78	B
	ATOM	1395	CB	LYS	B	311	66.419	44.014	42.471	1.00	30.98	B
	ATOM	1396	CG	LYS	B	311	67.876	44.355	42.676	1.00	34.65	B
50	ATOM	1397	CD	LYS	B	311	68.141	45.839	42.539	0.00	34.39	B
	ATOM	1398	CE	LYS	B	311	68.033	46.305	41.095	0.00	35.04	B
	ATOM	1399	NZ	LYS	B	311	66.665	46.176	40.520	0.00	35.23	B
	ATOM	1400	C	LYS	B	311	66.589	42.154	44.127	1.00	31.89	B
	ATOM	1401	O	LYS	B	311	67.761	41.815	44.325	1.00	31.11	B

	ATOM	1402	N	SER	B	312	65.666	42.181	45.088	1.00	32.44	B
	ATOM	1403	CA	SER	B	312	65.997	41.868	46.479	1.00	34.40	B
	ATOM	1404	CB	SER	B	312	64.998	42.541	47.433	1.00	35.97	B
	ATOM	1405	OG	SER	B	312	65.318	42.268	48.793	1.00	37.24	B
5	ATOM	1406	C	SER	B	312	66.068	40.389	46.825	1.00	33.58	B
	ATOM	1407	O	SER	B	312	65.154	39.629	46.532	1.00	35.14	B
	ATOM	1408	N	THR	B	313	67.160	39.990	47.460	1.00	32.17	B
	ATOM	1409	CA	THR	B	313	67.314	38.613	47.867	1.00	32.11	B
	ATOM	1410	CB	THR	B	313	68.760	38.142	47.682	1.00	34.02	B
10	ATOM	1411	OG1	THR	B	313	68.921	37.648	46.346	1.00	35.15	B
	ATOM	1412	CG2	THR	B	313	69.114	37.055	48.685	1.00	33.55	B
	ATOM	1413	C	THR	B	313	66.913	38.532	49.329	1.00	30.50	B
	ATOM	1414	O	THR	B	313	66.318	37.553	49.764	1.00	31.15	B
	ATOM	1415	N	SER	B	314	67.219	39.583	50.078	1.00	29.28	B
15	ATOM	1416	CA	SER	B	314	66.881	39.648	51.493	1.00	28.64	B
	ATOM	1417	CB	SER	B	314	67.307	40.990	52.076	1.00	28.48	B
	ATOM	1418	OG	SER	B	314	68.696	40.979	52.349	1.00	33.47	B
	ATOM	1419	C	SER	B	314	65.397	39.479	51.710	1.00	27.68	B
	ATOM	1420	O	SER	B	314	64.966	38.738	52.592	1.00	28.00	B
20	ATOM	1421	N	LEU	B	315	64.629	40.182	50.890	1.00	25.95	B
	ATOM	1422	CA	LEU	B	315	63.190	40.158	50.967	1.00	24.83	B
	ATOM	1423	CB	LEU	B	315	62.614	40.721	49.676	1.00	22.38	B
	ATOM	1424	CG	LEU	B	315	61.151	41.129	49.740	1.00	21.41	B
	ATOM	1425	CD1	LEU	B	315	61.006	42.400	50.604	1.00	20.01	B
25	ATOM	1426	CD2	LEU	B	315	60.662	41.376	48.345	1.00	19.89	B
	ATOM	1427	C	LEU	B	315	62.675	38.745	51.206	1.00	26.71	B
	ATOM	1428	O	LEU	B	315	61.894	38.494	52.141	1.00	27.54	B
	ATOM	1429	N	TRP	B	316	63.110	37.813	50.369	1.00	26.88	B
	ATOM	1430	CA	TRP	B	316	62.665	36.439	50.534	1.00	27.42	B
30	ATOM	1431	CB	TRP	B	316	62.776	35.691	49.204	1.00	27.04	B
	ATOM	1432	CG	TRP	B	316	62.021	36.416	48.176	1.00	25.52	B
	ATOM	1433	CD2	TRP	B	316	60.600	36.519	48.088	1.00	25.34	B
	ATOM	1434	CE2	TRP	B	316	60.313	37.456	47.071	1.00	24.36	B
	ATOM	1435	CE3	TRP	B	316	59.540	35.920	48.778	1.00	26.16	B
35	ATOM	1436	CD1	TRP	B	316	62.526	37.262	47.232	1.00	25.54	B
	ATOM	1437	NE1	TRP	B	316	61.507	37.892	46.566	1.00	23.85	B
	ATOM	1438	CZ2	TRP	B	316	59.003	37.808	46.728	1.00	23.50	B
	ATOM	1439	CZ3	TRP	B	316	58.236	36.272	48.438	1.00	24.82	B
	ATOM	1440	CH2	TRP	B	316	57.981	37.209	47.421	1.00	24.99	B
40	ATOM	1441	C	TRP	B	316	63.402	35.720	51.656	1.00	27.65	B
	ATOM	1442	O	TRP	B	316	62.786	34.989	52.446	1.00	27.76	B
	ATOM	1443	N	LYS	B	317	64.709	35.934	51.744	1.00	27.10	B
	ATOM	1444	CA	LYS	B	317	65.455	35.304	52.817	1.00	28.92	B
	ATOM	1445	CB	LYS	B	317	66.907	35.788	52.830	1.00	30.51	B
45	ATOM	1446	CG	LYS	B	317	67.768	35.175	53.935	1.00	32.68	B
	ATOM	1447	CD	LYS	B	317	69.209	35.655	53.820	1.00	35.89	B
	ATOM	1448	CE	LYS	B	317	69.849	35.839	55.186	1.00	37.32	B
	ATOM	1449	NZ	LYS	B	317	69.169	36.927	55.978	1.00	39.48	B
	ATOM	1450	C	LYS	B	317	64.764	35.597	54.164	1.00	29.21	B
50	ATOM	1451	O	LYS	B	317	64.560	34.682	54.975	1.00	28.72	B
	ATOM	1452	N	LYS	B	318	64.373	36.851	54.394	1.00	27.41	B
	ATOM	1453	CA	LYS	B	318	63.698	37.182	55.640	1.00	27.23	B
	ATOM	1454	CB	LYS	B	318	63.287	38.657	55.685	1.00	28.22	B
	ATOM	1455	CG	LYS	B	318	64.448	39.580	55.982	1.00	29.33	B

	ATOM	1456	CD	LYS	B	318	64.011	40.989	56.263	1.00	29.29	B
	ATOM	1457	CE	LYS	B	318	65.211	41.805	56.726	1.00	31.20	B
	ATOM	1458	NZ	LYS	B	318	66.332	41.748	55.749	1.00	29.62	B
	ATOM	1459	C	LYS	B	318	62.475	36.318	55.846	1.00	28.19	B
5	ATOM	1460	O	LYS	B	318	62.325	35.651	56.881	1.00	29.19	B
	ATOM	1461	N	LEU	B	319	61.598	36.346	54.847	1.00	28.31	B
	ATOM	1462	CA	LEU	B	319	60.353	35.576	54.851	1.00	26.08	B
	ATOM	1463	CB	LEU	B	319	59.644	35.756	53.499	1.00	24.60	B
	ATOM	1464	CG	LEU	B	319	58.949	37.106	53.299	1.00	23.31	B
10	ATOM	1465	CD1	LEU	B	319	58.929	37.501	51.828	1.00	25.42	B
	ATOM	1466	CD2	LEU	B	319	57.550	37.030	53.849	1.00	20.66	B
	ATOM	1467	C	LEU	B	319	60.661	34.104	55.115	1.00	24.68	B
	ATOM	1468	O	LEU	B	319	60.126	33.511	56.051	1.00	24.33	B
	ATOM	1469	N	LEU	B	320	61.521	33.515	54.292	1.00	24.37	B
15	ATOM	1470	CA	LEU	B	320	61.887	32.119	54.496	1.00	24.33	B
	ATOM	1471	CB	LEU	B	320	63.119	31.777	53.678	1.00	20.97	B
	ATOM	1472	CG	LEU	B	320	62.711	31.425	52.272	1.00	20.93	B
	ATOM	1473	CD1	LEU	B	320	63.945	31.333	51.431	1.00	21.63	B
	ATOM	1474	CD2	LEU	B	320	61.936	30.117	52.276	1.00	17.66	B
20	ATOM	1475	C	LEU	B	320	62.166	31.800	55.967	1.00	24.55	B
	ATOM	1476	O	LEU	B	320	61.744	30.769	56.491	1.00	25.31	B
	ATOM	1477	N	ILE	B	321	62.883	32.706	56.615	1.00	24.47	B
	ATOM	1478	CA	ILE	B	321	63.253	32.579	58.009	1.00	23.96	B
	ATOM	1479	CB	ILE	B	321	64.450	33.531	58.315	1.00	25.52	B
25	ATOM	1480	CG2	ILE	B	321	64.759	33.556	59.806	1.00	25.19	B
	ATOM	1481	CG1	ILE	B	321	65.671	33.094	57.498	1.00	23.92	B
	ATOM	1482	CD1	ILE	B	321	66.951	33.873	57.782	1.00	24.41	B
	ATOM	1483	C	ILE	B	321	62.065	32.882	58.928	1.00	23.22	B
	ATOM	1484	O	ILE	B	321	61.902	32.240	59.952	1.00	24.18	B
30	ATOM	1485	N	SER	B	322	61.239	33.853	58.563	1.00	23.04	B
	ATOM	1486	CA	SER	B	322	60.079	34.200	59.370	1.00	23.65	B
	ATOM	1487	CB	SER	B	322	59.248	35.266	58.670	1.00	21.62	B
	ATOM	1488	OG	SER	B	322	60.030	36.403	58.387	1.00	24.32	B
	ATOM	1489	C	SER	B	322	59.203	32.990	59.581	1.00	24.95	B
35	ATOM	1490	O	SER	B	322	58.789	32.691	60.696	1.00	28.00	B
	ATOM	1491	N	GLU	B	323	58.926	32.302	58.485	1.00	25.30	B
	ATOM	1492	CA	GLU	B	323	58.066	31.135	58.486	1.00	25.97	B
	ATOM	1493	CB	GLU	B	323	57.480	30.974	57.091	1.00	26.35	B
	ATOM	1494	CG	GLU	B	323	56.792	32.239	56.646	1.00	27.43	B
40	ATOM	1495	CD	GLU	B	323	55.441	32.431	57.307	1.00	27.80	B
	ATOM	1496	OE1	GLU	B	323	55.239	31.878	58.409	1.00	25.90	B
	ATOM	1497	OE2	GLU	B	323	54.590	33.142	56.718	1.00	28.13	B
	ATOM	1498	C	GLU	B	323	58.745	29.855	58.917	1.00	25.13	B
	ATOM	1499	O	GLU	B	323	58.123	28.792	58.931	1.00	25.20	B
45	ATOM	1500	N	ASN	B	324	60.019	29.966	59.276	1.00	24.08	B
	ATOM	1501	CA	ASN	B	324	60.808	28.816	59.708	1.00	24.96	B
	ATOM	1502	CB	ASN	B	324	60.203	28.185	60.974	1.00	26.02	B
	ATOM	1503	CG	ASN	B	324	60.051	29.187	62.108	1.00	28.82	B
	ATOM	1504	OD1	ASN	B	324	61.030	29.766	62.605	1.00	29.61	B
50	ATOM	1505	ND2	ASN	B	324	58.813	29.402	62.518	1.00	29.76	B
	ATOM	1506	C	ASN	B	324	60.906	27.776	58.588	1.00	24.92	B
	ATOM	1507	O	ASN	B	324	60.642	26.596	58.786	1.00	23.18	B
	ATOM	1508	N	PHE	B	325	61.269	28.226	57.395	1.00	25.71	B
	ATOM	1509	CA	PHE	B	325	61.406	27.304	56.287	1.00	25.91	B

	ATOM	1510	CB	PHE	B	325	60.839	27.913	55.008	1.00	24.25	B
	ATOM	1511	CG	PHE	B	325	59.334	27.935	54.987	1.00	23.73	B
	ATOM	1512	CD1	PHE	B	325	58.644	28.984	54.394	1.00	23.04	B
	ATOM	1513	CD2	PHE	B	325	58.604	26.925	55.616	1.00	20.21	B
5	ATOM	1514	CE1	PHE	B	325	57.259	29.025	54.437	1.00	20.96	B
	ATOM	1515	CE2	PHE	B	325	57.227	26.964	55.658	1.00	18.74	B
	ATOM	1516	CZ	PHE	B	325	56.555	28.015	55.073	1.00	19.51	B
	ATOM	1517	C	PHE	B	325	62.861	26.972	56.156	1.00	26.92	B
	ATOM	1518	O	PHE	B	325	63.232	26.019	55.478	1.00	28.62	B
10	ATOM	1519	N	VAL	B	326	63.683	27.766	56.833	1.00	27.50	B
	ATOM	1520	CA	VAL	B	326	65.127	27.577	56.849	1.00	27.18	B
	ATOM	1521	CB	VAL	B	326	65.773	28.060	55.532	1.00	25.75	B
	ATOM	1522	CG1	VAL	B	326	66.019	29.553	55.587	1.00	23.02	B
	ATOM	1523	CG2	VAL	B	326	67.061	27.316	55.288	1.00	26.04	B
15	ATOM	1524	C	VAL	B	326	65.685	28.408	57.993	1.00	28.22	B
	ATOM	1525	O	VAL	B	326	64.998	29.274	58.533	1.00	28.23	B
	ATOM	1526	N	SER	B	327	66.932	28.154	58.361	1.00	29.87	B
	ATOM	1527	CA	SER	B	327	67.547	28.926	59.427	1.00	32.04	B
	ATOM	1528	CB	SER	B	327	67.867	28.053	60.643	1.00	32.92	B
20	ATOM	1529	OG	SER	B	327	69.012	27.244	60.404	1.00	35.60	B
	ATOM	1530	C	SER	B	327	68.837	29.511	58.905	1.00	33.44	B
	ATOM	1531	O	SER	B	327	69.404	29.024	57.925	1.00	35.13	B
	ATOM	1532	N	PRO	B	328	69.328	30.561	59.568	1.00	34.95	B
	ATOM	1533	CD	PRO	B	328	68.703	31.277	60.698	1.00	34.72	B
25	ATOM	1534	CA	PRO	B	328	70.570	31.208	59.161	1.00	35.43	B
	ATOM	1535	CB	PRO	B	328	70.906	32.056	60.372	1.00	34.44	B
	ATOM	1536	CG	PRO	B	328	69.541	32.530	60.792	1.00	34.00	B
	ATOM	1537	C	PRO	B	328	71.674	30.211	58.789	1.00	37.33	B
	ATOM	1538	O	PRO	B	328	72.413	30.428	57.820	1.00	38.07	B
30	ATOM	1539	N	LYS	B	329	71.779	29.106	59.524	1.00	38.13	B
	ATOM	1540	CA	LYS	B	329	72.830	28.126	59.222	1.00	39.44	B
	ATOM	1541	CB	LYS	B	329	73.088	27.201	60.423	1.00	41.96	B
	ATOM	1542	CG	LYS	B	329	73.334	27.911	61.736	1.00	44.54	B
	ATOM	1543	CD	LYS	B	329	74.564	28.801	61.693	1.00	46.08	B
35	ATOM	1544	CE	LYS	B	329	74.745	29.475	63.047	1.00	47.88	B
	ATOM	1545	NZ	LYS	B	329	73.510	30.241	63.384	1.00	48.71	B
	ATOM	1546	C	LYS	B	329	72.539	27.255	58.005	1.00	38.23	B
	ATOM	1547	O	LYS	B	329	73.444	26.922	57.230	1.00	37.43	B
	ATOM	1548	N	GLY	B	330	71.279	26.863	57.858	1.00	36.83	B
40	ATOM	1549	CA	GLY	B	330	70.904	26.026	56.733	1.00	34.91	B
	ATOM	1550	C	GLY	B	330	70.671	26.809	55.458	1.00	33.34	B
	ATOM	1551	O	GLY	B	330	70.432	26.217	54.402	1.00	31.96	B
	ATOM	1552	N	PHE	B	331	70.742	28.136	55.554	1.00	32.27	B
	ATOM	1553	CA	PHE	B	331	70.517	28.977	54.388	1.00	32.81	B
45	ATOM	1554	CB	PHE	B	331	70.778	30.454	54.688	1.00	32.71	B
	ATOM	1555	CG	PHE	B	331	70.365	31.374	53.561	1.00	35.02	B
	ATOM	1556	CD1	PHE	B	331	69.013	31.631	53.319	1.00	34.88	B
	ATOM	1557	CD2	PHE	B	331	71.323	31.971	52.727	1.00	36.79	B
	ATOM	1558	CE1	PHE	B	331	68.609	32.466	52.274	1.00	35.03	B
50	ATOM	1559	CE2	PHE	B	331	70.933	32.816	51.670	1.00	36.82	B
	ATOM	1560	CZ	PHE	B	331	69.568	33.061	51.446	1.00	36.85	B
	ATOM	1561	C	PHE	B	331	71.333	28.600	53.164	1.00	32.72	B
	ATOM	1562	O	PHE	B	331	70.779	28.197	52.143	1.00	32.53	B
	ATOM	1563	N	ASN	B	332	72.650	28.725	53.261	1.00	33.63	B

5	ATOM	1564	CA	ASN	B	332	73.495	28.430	52.116	1.00	34.96	B
	ATOM	1565	CB	ASN	B	332	74.956	28.510	52.503	1.00	35.07	B
	ATOM	1566	CG	ASN	B	332	75.386	29.925	52.769	1.00	36.45	B
	ATOM	1567	OD1	ASN	B	332	74.860	30.864	52.165	1.00	36.09	B
	ATOM	1568	ND2	ASN	B	332	76.352	30.096	53.666	1.00	37.34	B
	ATOM	1569	C	ASN	B	332	73.204	27.105	51.457	1.00	35.37	B
	ATOM	1570	O	ASN	B	332	73.006	27.034	50.240	1.00	34.82	B
	ATOM	1571	N	SER	B	333	73.174	26.050	52.253	1.00	36.35	B
10	ATOM	1572	CA	SER	B	333	72.897	24.749	51.696	1.00	38.23	B
	ATOM	1573	CB	SER	B	333	72.767	23.724	52.804	1.00	37.83	B
	ATOM	1574	OG	SER	B	333	72.509	22.458	52.236	1.00	43.08	B
	ATOM	1575	C	SER	B	333	71.615	24.785	50.867	1.00	38.81	B
	ATOM	1576	O	SER	B	333	71.522	24.144	49.814	1.00	39.26	B
15	ATOM	1577	N	LEU	B	334	70.629	25.533	51.357	1.00	38.86	B
	ATOM	1578	CA	LEU	B	334	69.338	25.688	50.685	1.00	37.16	B
	ATOM	1579	CB	LEU	B	334	68.446	26.645	51.486	1.00	34.21	B
	ATOM	1580	CG	LEU	B	334	67.149	27.126	50.830	1.00	33.30	B
	ATOM	1581	CD1	LEU	B	334	66.189	25.957	50.642	1.00	29.33	B
20	ATOM	1582	CD2	LEU	B	334	66.528	28.209	51.688	1.00	31.65	B
	ATOM	1583	C	LEU	B	334	69.574	26.251	49.291	1.00	37.44	B
	ATOM	1584	O	LEU	B	334	69.105	25.700	48.293	1.00	36.40	B
	ATOM	1585	N	ASN	B	335	70.306	27.361	49.248	1.00	38.10	B
	ATOM	1586	CA	ASN	B	335	70.647	28.032	48.001	1.00	38.02	B
25	ATOM	1587	CB	ASN	B	335	71.590	29.188	48.289	1.00	37.88	B
	ATOM	1588	CG	ASN	B	335	70.871	30.496	48.329	1.00	40.34	B
	ATOM	1589	OD1	ASN	B	335	71.266	31.422	49.033	1.00	43.76	B
	ATOM	1590	ND2	ASN	B	335	69.800	30.591	47.556	1.00	41.28	B
	ATOM	1591	C	ASN	B	335	71.292	27.070	47.013	1.00	38.24	B
30	ATOM	1592	O	ASN	B	335	70.906	27.003	45.847	1.00	38.64	B
	ATOM	1593	N	LEU	B	336	72.274	26.325	47.498	1.00	36.78	B
	ATOM	1594	CA	LEU	B	336	72.978	25.364	46.683	1.00	35.71	B
	ATOM	1595	CB	LEU	B	336	74.041	24.658	47.522	1.00	35.78	B
	ATOM	1596	CG	LEU	B	336	74.991	23.682	46.827	1.00	35.54	B
35	ATOM	1597	CD1	LEU	B	336	75.977	24.436	45.942	1.00	35.55	B
	ATOM	1598	CD2	LEU	B	336	75.716	22.899	47.883	1.00	36.31	B
	ATOM	1599	C	LEU	B	336	71.997	24.336	46.123	1.00	35.77	B
	ATOM	1600	O	LEU	B	336	72.075	23.961	44.954	1.00	37.71	B
	ATOM	1601	N	LYS	B	337	71.068	23.876	46.953	1.00	34.49	B
40	ATOM	1602	CA	LYS	B	337	70.097	22.878	46.508	1.00	31.85	B
	ATOM	1603	CB	LYS	B	337	69.310	22.320	47.704	1.00	30.25	B
	ATOM	1604	CG	LYS	B	337	68.298	21.237	47.321	1.00	32.14	B
	ATOM	1605	CD	LYS	B	337	67.438	20.697	48.512	1.00	35.02	B
	ATOM	1606	CE	LYS	B	337	66.544	21.789	49.173	1.00	35.41	B
45	ATOM	1607	NZ	LYS	B	337	65.466	21.260	50.081	1.00	32.74	B
	ATOM	1608	C	LYS	B	337	69.129	23.433	45.461	1.00	30.95	B
	ATOM	1609	O	LYS	B	337	68.793	22.740	44.519	1.00	29.84	B
	ATOM	1610	N	LEU	B	338	68.690	24.679	45.636	1.00	31.30	B
	ATOM	1611	CA	LEU	B	338	67.755	25.324	44.714	1.00	30.02	B
50	ATOM	1612	CB	LEU	B	338	67.218	26.621	45.317	1.00	29.04	B
	ATOM	1613	CG	LEU	B	338	66.157	26.563	46.434	1.00	29.18	B
	ATOM	1614	CD1	LEU	B	338	65.834	27.996	46.909	1.00	25.48	B
	ATOM	1615	CD2	LEU	B	338	64.897	25.881	45.919	1.00	26.03	B
	ATOM	1616	C	LEU	B	338	68.433	25.639	43.400	1.00	30.20	B
	ATOM	1617	O	LEU	B	338	67.809	25.643	42.340	1.00	29.78	B

	ATOM	1618	N	SER	B	339	69.724	25.918	43.487	1.00	30.16	B
	ATOM	1619	CA	SER	B	339	70.510	26.227	42.317	1.00	29.06	B
	ATOM	1620	CB	SER	B	339	71.913	26.656	42.712	1.00	27.05	B
	ATOM	1621	OG	SER	B	339	72.665	26.965	41.560	1.00	25.97	B
5	ATOM	1622	C	SER	B	339	70.598	24.979	41.483	1.00	30.90	B
	ATOM	1623	O	SER	B	339	70.580	25.029	40.254	1.00	32.89	B
	ATOM	1624	N	GLN	B	340	70.701	23.842	42.149	1.00	30.57	B
	ATOM	1625	CA	GLN	B	340	70.796	22.605	41.409	1.00	31.13	B
	ATOM	1626	CB	GLN	B	340	71.238	21.496	42.334	1.00	32.53	B
10	ATOM	1627	CG	GLN	B	340	72.619	21.768	42.867	1.00	35.89	B
	ATOM	1628	CD	GLN	B	340	73.040	20.758	43.900	1.00	36.30	B
	ATOM	1629	OE1	GLN	B	340	72.209	19.975	44.393	1.00	37.07	B
	ATOM	1630	NE2	GLN	B	340	74.332	20.765	44.248	1.00	34.68	B
	ATOM	1631	C	GLN	B	340	69.471	22.276	40.774	1.00	31.71	B
15	ATOM	1632	O	GLN	B	340	69.418	21.644	39.726	1.00	32.80	B
	ATOM	1633	N	LYS	B	341	68.403	22.738	41.408	1.00	32.39	B
	ATOM	1634	CA	LYS	B	341	67.047	22.505	40.942	1.00	33.18	B
	ATOM	1635	CB	LYS	B	341	66.086	22.760	42.094	1.00	34.86	B
	ATOM	1636	CG	LYS	B	341	64.697	22.223	41.889	1.00	38.21	B
20	ATOM	1637	CD	LYS	B	341	63.793	22.574	43.061	1.00	40.03	B
	ATOM	1638	CE	LYS	B	341	62.406	21.980	42.836	1.00	42.58	B
	ATOM	1639	NZ	LYS	B	341	61.380	22.609	43.719	1.00	42.83	B
	ATOM	1640	C	LYS	B	341	66.661	23.392	39.764	1.00	34.36	B
	ATOM	1641	O	LYS	B	341	66.041	22.939	38.805	1.00	34.14	B
25	ATOM	1642	N	TYR	B	342	67.043	24.658	39.857	1.00	34.90	B
	ATOM	1643	CA	TYR	B	342	66.734	25.660	38.853	1.00	35.01	B
	ATOM	1644	CB	TYR	B	342	65.844	26.695	39.497	1.00	37.87	B
	ATOM	1645	CG	TYR	B	342	64.647	26.082	40.153	1.00	41.65	B
	ATOM	1646	CD1	TYR	B	342	63.646	25.507	39.384	1.00	42.60	B
30	ATOM	1647	CE1	TYR	B	342	62.525	24.958	39.968	1.00	45.40	B
	ATOM	1648	CD2	TYR	B	342	64.501	26.088	41.538	1.00	42.64	B
	ATOM	1649	CE2	TYR	B	342	63.376	25.540	42.139	1.00	44.31	B
	ATOM	1650	CZ	TYR	B	342	62.386	24.978	41.343	1.00	45.73	B
	ATOM	1651	OH	TYR	B	342	61.232	24.462	41.896	1.00	46.50	B
35	ATOM	1652	C	TYR	B	342	67.991	26.339	38.343	1.00	34.71	B
	ATOM	1653	O	TYR	B	342	68.287	27.467	38.729	1.00	35.57	B
	ATOM	1654	N	PRO	B	343	68.754	25.663	37.474	1.00	34.09	B
	ATOM	1655	CD	PRO	B	343	68.568	24.298	36.955	1.00	33.06	B
	ATOM	1656	CA	PRO	B	343	69.982	26.256	36.942	1.00	34.15	B
40	ATOM	1657	CB	PRO	B	343	70.427	25.231	35.902	1.00	32.61	B
	ATOM	1658	CG	PRO	B	343	69.940	23.953	36.458	1.00	30.81	B
	ATOM	1659	C	PRO	B	343	69.805	27.655	36.332	1.00	34.54	B
	ATOM	1660	O	PRO	B	343	70.562	28.577	36.639	1.00	34.01	B
	ATOM	1661	N	LYS	B	344	68.793	27.803	35.483	1.00	34.28	B
45	ATOM	1662	CA	LYS	B	344	68.537	29.063	34.799	1.00	34.41	B
	ATOM	1663	CB	LYS	B	344	67.823	28.791	33.483	1.00	34.70	B
	ATOM	1664	CG	LYS	B	344	68.487	27.758	32.623	1.00	32.84	B
	ATOM	1665	CD	LYS	B	344	67.566	27.409	31.505	1.00	32.13	B
	ATOM	1666	CE	LYS	B	344	67.769	25.984	31.078	1.00	32.95	B
50	ATOM	1667	NZ	LYS	B	344	66.694	25.581	30.144	1.00	35.30	B
	ATOM	1668	C	LYS	B	344	67.778	30.156	35.547	1.00	34.52	B
	ATOM	1669	O	LYS	B	344	67.446	31.188	34.950	1.00	33.51	B
	ATOM	1670	N	LEU	B	345	67.475	29.921	36.825	1.00	32.93	B
	ATOM	1671	CA	LEU	B	345	66.792	30.916	37.663	1.00	30.85	B

5	ATOM	1672	CB	LEU	B	345	65.856	30.253	38.660	1.00	28.33	B
	ATOM	1673	CG	LEU	B	345	64.506	29.850	38.111	1.00	27.26	B
	ATOM	1674	CD1	LEU	B	345	63.691	29.121	39.179	1.00	24.62	B
	ATOM	1675	CD2	LEU	B	345	63.804	31.102	37.655	1.00	26.44	B
	ATOM	1676	C	LEU	B	345	67.834	31.674	38.440	1.00	31.07	B
10	ATOM	1677	O	LEU	B	345	68.961	31.210	38.580	1.00	31.79	B
	ATOM	1678	N	SER	B	346	67.458	32.830	38.970	1.00	33.11	B
	ATOM	1679	CA	SER	B	346	68.392	33.653	39.754	1.00	34.10	B
	ATOM	1680	CB	SER	B	346	68.283	35.114	39.349	1.00	34.20	B
	ATOM	1681	OG	SER	B	346	67.035	35.623	39.779	1.00	37.09	B
15	ATOM	1682	C	SER	B	346	68.098	33.563	41.247	1.00	33.12	B
	ATOM	1683	O	SER	B	346	66.971	33.302	41.655	1.00	33.78	B
	ATOM	1684	N	GLN	B	347	69.113	33.814	42.056	1.00	32.28	B
	ATOM	1685	CA	GLN	B	347	68.950	33.749	43.495	1.00	32.88	B
	ATOM	1686	CB	GLN	B	347	70.071	34.502	44.177	1.00	33.73	B
20	ATOM	1687	CG	GLN	B	347	70.009	34.451	45.667	1.00	33.40	B
	ATOM	1688	CD	GLN	B	347	71.105	35.276	46.251	1.00	36.19	B
	ATOM	1689	OE1	GLN	B	347	71.164	36.494	46.031	1.00	38.25	B
	ATOM	1690	NE2	GLN	B	347	72.006	34.627	46.984	1.00	36.38	B
	ATOM	1691	C	GLN	B	347	67.620	34.314	43.973	1.00	31.82	B
25	ATOM	1692	O	GLN	B	347	66.834	33.616	44.620	1.00	31.26	B
	ATOM	1693	N	GLN	B	348	67.370	35.581	43.661	1.00	30.61	B
	ATOM	1694	CA	GLN	B	348	66.121	36.195	44.076	1.00	30.85	B
	ATOM	1695	CB	GLN	B	348	65.984	37.626	43.542	1.00	31.61	B
	ATOM	1696	CG	GLN	B	348	67.092	38.583	43.958	1.00	31.41	B
30	ATOM	1697	CD	GLN	B	348	68.291	38.552	43.014	1.00	30.33	B
	ATOM	1698	OE1	GLN	B	348	69.055	39.512	42.942	1.00	29.04	B
	ATOM	1699	NE2	GLN	B	348	68.461	37.452	42.296	1.00	29.86	B
	ATOM	1700	C	GLN	B	348	64.942	35.364	43.593	1.00	29.45	B
	ATOM	1701	O	GLN	B	348	64.183	34.831	44.400	1.00	28.92	B
35	ATOM	1702	N	ASP	B	349	64.776	35.236	42.283	1.00	28.60	B
	ATOM	1703	CA	ASP	B	349	63.646	34.458	41.805	1.00	27.39	B
	ATOM	1704	CB	ASP	B	349	63.631	34.372	40.282	1.00	28.50	B
	ATOM	1705	CG	ASP	B	349	63.164	35.666	39.632	1.00	30.39	B
	ATOM	1706	OD1	ASP	B	349	62.212	36.306	40.153	1.00	29.22	B
40	ATOM	1707	OD2	ASP	B	349	63.744	36.034	38.590	1.00	31.83	B
	ATOM	1708	C	ASP	B	349	63.571	33.061	42.404	1.00	25.37	B
	ATOM	1709	O	ASP	B	349	62.476	32.546	42.597	1.00	24.91	B
	ATOM	1710	N	ARG	B	350	64.720	32.454	42.695	1.00	22.81	B
	ATOM	1711	CA	ARG	B	350	64.746	31.117	43.280	1.00	21.59	B
45	ATOM	1712	CB	ARG	B	350	66.178	30.611	43.428	1.00	23.28	B
	ATOM	1713	CG	ARG	B	350	66.787	30.106	42.133	1.00	27.24	B
	ATOM	1714	CD	ARG	B	350	68.195	29.544	42.333	1.00	26.74	B
	ATOM	1715	NE	ARG	B	350	68.820	29.271	41.051	1.00	27.71	B
	ATOM	1716	CZ	ARG	B	350	70.128	29.218	40.860	1.00	29.79	B
50	ATOM	1717	NH1	ARG	B	350	70.956	29.416	41.878	1.00	31.36	B
	ATOM	1718	NH2	ARG	B	350	70.604	28.990	39.642	1.00	31.57	B
	ATOM	1719	C	ARG	B	350	64.094	31.124	44.651	1.00	20.94	B
	ATOM	1720	O	ARG	B	350	63.103	30.429	44.893	1.00	20.47	B
	ATOM	1721	N	LEU	B	351	64.672	31.909	45.549	1.00	18.79	B
50	ATOM	1722	CA	LEU	B	351	64.157	32.026	46.890	1.00	17.44	B
	ATOM	1723	CB	LEU	B	351	64.895	33.143	47.624	1.00	14.47	B
	ATOM	1724	CG	LEU	B	351	66.358	32.799	47.897	1.00	14.78	B
	ATOM	1725	CD1	LEU	B	351	66.992	33.900	48.730	1.00	17.09	B

	ATOM	1726	CD2	LEU	B	351	66.466	31.467	48.619	1.00	12.98	B
	ATOM	1727	C	LEU	B	351	62.638	32.247	46.942	1.00	18.50	B
	ATOM	1728	O	LEU	B	351	61.958	31.715	47.826	1.00	17.10	B
	ATOM	1729	N	ARG	B	352	62.092	33.003	45.995	1.00	18.20	B
5	ATOM	1730	CA	ARG	B	352	60.652	33.246	45.997	1.00	20.70	B
	ATOM	1731	CB	ARG	B	352	60.301	34.404	45.060	1.00	22.90	B
	ATOM	1732	CG	ARG	B	352	58.821	34.519	44.704	1.00	21.25	B
	ATOM	1733	CD	ARG	B	352	58.577	35.861	44.037	1.00	24.96	B
	ATOM	1734	NE	ARG	B	352	59.336	36.027	42.793	1.00	26.60	B
10	ATOM	1735	CZ	ARG	B	352	58.840	35.772	41.588	1.00	24.08	B
	ATOM	1736	NH1	ARG	B	352	57.589	35.344	41.468	1.00	25.95	B
	ATOM	1737	NH2	ARG	B	352	59.582	35.955	40.508	1.00	23.94	B
	ATOM	1738	C	ARG	B	352	59.868	32.014	45.590	1.00	20.80	B
	ATOM	1739	O	ARG	B	352	58.812	31.701	46.151	1.00	20.69	B
15	ATOM	1740	N	LEU	B	353	60.385	31.308	44.601	1.00	22.07	B
	ATOM	1741	CA	LEU	B	353	59.703	30.115	44.135	1.00	24.32	B
	ATOM	1742	CB	LEU	B	353	60.494	29.510	42.971	1.00	24.67	B
	ATOM	1743	CG	LEU	B	353	59.774	28.524	42.058	1.00	26.68	B
	ATOM	1744	CD1	LEU	B	353	59.623	27.208	42.767	1.00	28.84	B
20	ATOM	1745	CD2	LEU	B	353	58.420	29.098	41.635	1.00	28.75	B
	ATOM	1746	C	LEU	B	353	59.614	29.166	45.336	1.00	25.14	B
	ATOM	1747	O	LEU	B	353	58.568	28.566	45.604	1.00	24.06	B
	ATOM	1748	N	SER	B	354	60.728	29.085	46.063	1.00	25.53	B
	ATOM	1749	CA	SER	B	354	60.867	28.264	47.262	1.00	26.14	B
25	ATOM	1750	CB	SER	B	354	62.273	28.450	47.849	1.00	25.96	B
	ATOM	1751	OG	SER	B	354	62.454	27.730	49.061	1.00	23.97	B
	ATOM	1752	C	SER	B	354	59.830	28.656	48.313	1.00	27.19	B
	ATOM	1753	O	SER	B	354	59.098	27.818	48.837	1.00	27.24	B
	ATOM	1754	N	PHE	B	355	59.769	29.941	48.625	1.00	27.04	B
30	ATOM	1755	CA	PHE	B	355	58.822	30.390	49.616	1.00	26.23	B
	ATOM	1756	CB	PHE	B	355	58.954	31.882	49.854	1.00	27.13	B
	ATOM	1757	CG	PHE	B	355	58.041	32.400	50.920	1.00	26.97	B
	ATOM	1758	CD1	PHE	B	355	56.736	32.763	50.626	1.00	26.60	B
	ATOM	1759	CD2	PHE	B	355	58.495	32.522	52.228	1.00	28.32	B
35	ATOM	1760	CE1	PHE	B	355	55.892	33.236	51.626	1.00	27.60	B
	ATOM	1761	CE2	PHE	B	355	57.661	32.992	53.237	1.00	26.91	B
	ATOM	1762	CZ	PHE	B	355	56.360	33.353	52.934	1.00	27.81	B
	ATOM	1763	C	PHE	B	355	57.413	30.087	49.203	1.00	25.95	B
	ATOM	1764	O	PHE	B	355	56.687	29.427	49.929	1.00	25.86	B
40	ATOM	1765	N	LEU	B	356	57.015	30.575	48.037	1.00	27.00	B
	ATOM	1766	CA	LEU	B	356	55.655	30.337	47.570	1.00	27.63	B
	ATOM	1767	CB	LEU	B	356	55.487	30.886	46.144	1.00	28.43	B
	ATOM	1768	CG	LEU	B	356	55.485	32.412	45.923	1.00	28.92	B
	ATOM	1769	CD1	LEU	B	356	55.449	32.704	44.421	1.00	28.25	B
45	ATOM	1770	CD2	LEU	B	356	54.299	33.063	46.620	1.00	26.99	B
	ATOM	1771	C	LEU	B	356	55.297	28.842	47.618	1.00	26.51	B
	ATOM	1772	O	LEU	B	356	54.170	28.492	47.910	1.00	25.42	B
	ATOM	1773	N	GLU	B	357	56.267	27.976	47.343	1.00	27.82	B
	ATOM	1774	CA	GLU	B	357	56.051	26.537	47.357	1.00	28.89	B
50	ATOM	1775	CB	GLU	B	357	57.223	25.841	46.668	1.00	30.18	B
	ATOM	1776	CG	GLU	B	357	57.193	24.319	46.727	1.00	34.82	B
	ATOM	1777	CD	GLU	B	357	58.032	23.659	45.640	1.00	38.48	B
	ATOM	1778	OE1	GLU	B	357	59.254	23.926	45.569	1.00	41.06	B
	ATOM	1779	OE2	GLU	B	357	57.460	22.870	44.849	1.00	40.28	B

	ATOM	1780	C	GLU	B	357	55.899	26.016	48.790	1.00	29.56	B
	ATOM	1781	O	GLU	B	357	55.055	25.165	49.072	1.00	30.56	B
	ATOM	1782	N	ASN	B	358	56.722	26.529	49.692	1.00	27.38	B
	ATOM	1783	CA	ASN	B	358	56.659	26.124	51.072	1.00	26.16	B
5	ATOM	1784	CB	ASN	B	358	57.913	26.583	51.804	1.00	24.91	B
	ATOM	1785	CG	ASN	B	358	58.964	25.505	51.866	1.00	24.24	B
	ATOM	1786	OD1	ASN	B	358	60.149	25.794	51.827	1.00	24.48	B
	ATOM	1787	ND2	ASN	B	358	58.530	24.242	51.976	1.00	23.61	B
	ATOM	1788	C	ASN	B	358	55.440	26.669	51.796	1.00	27.01	B
10	ATOM	1789	O	ASN	B	358	54.743	25.940	52.500	1.00	29.45	B
	ATOM	1790	N	ILE	B	359	55.169	27.948	51.603	1.00	25.54	B
	ATOM	1791	CA	ILE	B	359	54.066	28.576	52.287	1.00	24.86	B
	ATOM	1792	CB	ILE	B	359	53.989	30.111	51.964	1.00	23.57	B
	ATOM	1793	CG2	ILE	B	359	53.438	30.361	50.544	1.00	22.38	B
15	ATOM	1794	CG1	ILE	B	359	53.099	30.808	52.994	1.00	21.88	B
	ATOM	1795	CD1	ILE	B	359	53.627	30.735	54.428	1.00	17.84	B
	ATOM	1796	C	ILE	B	359	52.726	27.929	51.992	1.00	27.18	B
	ATOM	1797	O	ILE	B	359	51.864	27.842	52.859	1.00	27.37	B
	ATOM	1798	N	PHE	B	360	52.533	27.457	50.775	1.00	29.04	B
20	ATOM	1799	CA	PHE	B	360	51.260	26.850	50.480	1.00	30.13	B
	ATOM	1800	CB	PHE	B	360	50.977	26.994	48.976	1.00	31.09	B
	ATOM	1801	CG	PHE	B	360	50.729	28.441	48.552	1.00	35.13	B
	ATOM	1802	CD1	PHE	B	360	49.750	29.214	49.196	1.00	36.04	B
	ATOM	1803	CD2	PHE	B	360	51.480	29.040	47.540	1.00	35.99	B
25	ATOM	1804	CE1	PHE	B	360	49.531	30.554	48.837	1.00	36.47	B
	ATOM	1805	CE2	PHE	B	360	51.265	30.380	47.177	1.00	37.16	B
	ATOM	1806	CZ	PHE	B	360	50.290	31.138	47.827	1.00	35.98	B
	ATOM	1807	C	PHE	B	360	51.137	25.414	51.019	1.00	28.89	B
	ATOM	1808	O	PHE	B	360	50.040	24.932	51.282	1.00	29.91	B
30	ATOM	1809	N	ILE	B	361	52.258	24.739	51.221	1.00	26.91	B
	ATOM	1810	CA	ILE	B	361	52.212	23.405	51.799	1.00	25.90	B
	ATOM	1811	CB	ILE	B	361	53.567	22.687	51.626	1.00	24.75	B
	ATOM	1812	CG2	ILE	B	361	53.707	21.556	52.648	1.00	20.19	B
	ATOM	1813	CG1	ILE	B	361	53.695	22.198	50.187	1.00	21.38	B
35	ATOM	1814	CD1	ILE	B	361	55.017	21.579	49.880	1.00	21.49	B
	ATOM	1815	C	ILE	B	361	51.894	23.539	53.303	1.00	25.76	B
	ATOM	1816	O	ILE	B	361	51.165	22.724	53.854	1.00	25.25	B
	ATOM	1817	N	LEU	B	362	52.455	24.558	53.955	1.00	24.78	B
	ATOM	1818	CA	LEU	B	362	52.200	24.780	55.367	1.00	24.80	B
40	ATOM	1819	CB	LEU	B	362	53.097	25.890	55.942	1.00	24.95	B
	ATOM	1820	CG	LEU	B	362	52.861	26.232	57.439	1.00	25.61	B
	ATOM	1821	CD1	LEU	B	362	53.251	25.034	58.290	1.00	23.05	B
	ATOM	1822	CD2	LEU	B	362	53.682	27.448	57.891	1.00	24.66	B
	ATOM	1823	C	LEU	B	362	50.746	25.192	55.479	1.00	24.68	B
45	ATOM	1824	O	LEU	B	362	50.075	24.847	56.440	1.00	25.14	B
	ATOM	1825	N	LYS	B	363	50.262	25.932	54.485	1.00	26.90	B
	ATOM	1826	CA	LYS	B	363	48.870	26.397	54.455	1.00	28.18	B
	ATOM	1827	CB	LYS	B	363	48.607	27.192	53.178	1.00	30.22	B
	ATOM	1828	CG	LYS	B	363	48.946	28.677	53.262	1.00	34.21	B
50	ATOM	1829	CD	LYS	B	363	47.787	29.466	53.860	1.00	35.29	B
	ATOM	1830	CE	LYS	B	363	48.036	30.984	53.859	1.00	38.15	B
	ATOM	1831	NZ	LYS	B	363	48.196	31.608	52.486	1.00	38.16	B
	ATOM	1832	C	LYS	B	363	47.931	25.209	54.497	1.00	27.14	B
	ATOM	1833	O	LYS	B	363	46.852	25.288	55.076	1.00	27.91	B

	ATOM	1834	N	ASN	B	364	48.365	24.119	53.872	1.00	26.50	B
	ATOM	1835	CA	ASN	B	364	47.602	22.893	53.809	1.00	28.02	B
	ATOM	1836	CB	ASN	B	364	48.119	21.990	52.692	1.00	29.30	B
	ATOM	1837	CG	ASN	B	364	47.742	22.485	51.311	1.00	30.37	B
5	ATOM	1838	OD1	ASN	B	364	48.127	21.882	50.299	1.00	29.53	B
	ATOM	1839	ND2	ASN	B	364	46.982	23.584	51.255	1.00	31.60	B
	ATOM	1840	C	ASN	B	364	47.696	22.129	55.106	1.00	27.69	B
	ATOM	1841	O	ASN	B	364	46.716	21.551	55.559	1.00	28.47	B
	ATOM	1842	N	TRP	B	365	48.882	22.093	55.693	1.00	26.51	B
10	ATOM	1843	CA	TRP	B	365	49.039	21.371	56.938	1.00	27.73	B
	ATOM	1844	CB	TRP	B	365	50.489	21.397	57.400	1.00	29.20	B
	ATOM	1845	CG	TRP	B	365	51.351	20.381	56.790	1.00	29.13	B
	ATOM	1846	CD2	TRP	B	365	51.742	19.142	57.379	1.00	29.19	B
	ATOM	1847	CE2	TRP	B	365	52.638	18.523	56.489	1.00	28.54	B
15	ATOM	1848	CE3	TRP	B	365	51.425	18.495	58.579	1.00	29.88	B
	ATOM	1849	CD1	TRP	B	365	51.989	20.460	55.598	1.00	28.45	B
	ATOM	1850	NE1	TRP	B	365	52.771	19.351	55.406	1.00	27.81	B
	ATOM	1851	CZ2	TRP	B	365	53.230	17.282	56.758	1.00	28.80	B
	ATOM	1852	CZ3	TRP	B	365	52.018	17.257	58.842	1.00	29.52	B
20	ATOM	1853	CH2	TRP	B	365	52.909	16.671	57.934	1.00	27.59	B
	ATOM	1854	C	TRP	B	365	48.183	21.976	58.037	1.00	27.25	B
	ATOM	1855	O	TRP	B	365	47.686	21.262	58.898	1.00	27.54	B
	ATOM	1856	N	TYR	B	366	48.015	23.293	57.985	1.00	25.59	B
	ATOM	1857	CA	TYR	B	366	47.271	24.038	58.989	1.00	25.83	B
25	ATOM	1858	CB	TYR	B	366	47.858	25.433	59.127	1.00	24.61	B
	ATOM	1859	CG	TYR	B	366	49.220	25.559	59.761	1.00	22.97	B
	ATOM	1860	CD1	TYR	B	366	49.803	24.511	60.469	1.00	23.61	B
	ATOM	1861	CE1	TYR	B	366	50.999	24.699	61.170	1.00	21.04	B
	ATOM	1862	CD2	TYR	B	366	49.871	26.779	59.760	1.00	21.89	B
30	ATOM	1863	CE2	TYR	B	366	51.050	26.968	60.452	1.00	20.89	B
	ATOM	1864	CZ	TYR	B	366	51.603	25.940	61.153	1.00	20.92	B
	ATOM	1865	OH	TYR	B	366	52.741	26.179	61.878	1.00	21.34	B
	ATOM	1866	C	TYR	B	366	45.781	24.205	58.730	1.00	26.75	B
	ATOM	1867	O	TYR	B	366	45.053	24.659	59.618	1.00	25.47	B
35	ATOM	1868	N	ASN	B	367	45.343	23.874	57.516	1.00	27.78	B
	ATOM	1869	CA	ASN	B	367	43.935	23.993	57.137	1.00	28.96	B
	ATOM	1870	CB	ASN	B	367	43.789	24.062	55.611	1.00	27.81	B
	ATOM	1871	CG	ASN	B	367	42.420	24.542	55.172	1.00	27.70	B
	ATOM	1872	OD1	ASN	B	367	41.462	24.533	55.944	1.00	29.38	B
40	ATOM	1873	ND2	ASN	B	367	42.321	24.957	53.915	1.00	27.06	B
	ATOM	1874	C	ASN	B	367	43.184	22.772	57.668	1.00	29.83	B
	ATOM	1875	O	ASN	B	367	43.454	21.638	57.253	1.00	30.52	B
	ATOM	1876	N	PRO	B	368	42.246	22.988	58.613	1.00	30.10	B
	ATOM	1877	CD	PRO	B	368	41.884	24.278	59.227	1.00	28.86	B
45	ATOM	1878	CA	PRO	B	368	41.458	21.889	59.200	1.00	29.62	B
	ATOM	1879	CB	PRO	B	368	40.654	22.578	60.304	1.00	28.09	B
	ATOM	1880	CG	PRO	B	368	41.398	23.839	60.573	1.00	28.33	B
	ATOM	1881	C	PRO	B	368	40.534	21.318	58.133	1.00	29.34	B
	ATOM	1882	O	PRO	B	368	40.223	20.133	58.118	1.00	28.44	B
50	ATOM	1883	N	LYS	B	369	40.083	22.202	57.256	1.00	29.08	B
	ATOM	1884	CA	LYS	B	369	39.202	21.814	56.187	1.00	30.72	B
	ATOM	1885	CB	LYS	B	369	38.417	23.044	55.697	1.00	32.78	B
	ATOM	1886	CG	LYS	B	369	37.095	23.310	56.487	1.00	34.07	B
	ATOM	1887	CD	LYS	B	369	36.649	24.778	56.462	1.00	36.76	B

	ATOM	1888	CE	LYS	B	369	36.882	25.442	55.098	1.00	38.43	B
	ATOM	1889	NZ	LYS	B	369	36.568	26.906	55.151	1.00	41.21	B
	ATOM	1890	C	LYS	B	369	39.977	21.145	55.050	1.00	30.60	B
	ATOM	1891	O	LYS	B	369	39.389	20.779	54.040	1.00	32.44	B
5	ATOM	1892	N	PHE	B	370	41.293	20.985	55.207	1.00	29.96	B
	ATOM	1893	CA	PHE	B	370	42.111	20.335	54.175	1.00	28.15	B
	ATOM	1894	CB	PHE	B	370	43.422	21.107	53.934	1.00	29.31	B
	ATOM	1895	CG	PHE	B	370	44.447	20.330	53.124	1.00	31.81	B
	ATOM	1896	CD1	PHE	B	370	45.283	19.394	53.738	1.00	34.71	B
10	ATOM	1897	CD2	PHE	B	370	44.536	20.484	51.745	1.00	31.92	B
	ATOM	1898	CE1	PHE	B	370	46.185	18.625	52.992	1.00	34.80	B
	ATOM	1899	CE2	PHE	B	370	45.436	19.718	50.992	1.00	33.21	B
	ATOM	1900	CZ	PHE	B	370	46.259	18.785	51.622	1.00	33.35	B
	ATOM	1901	C	PHE	B	370	42.431	18.886	54.537	1.00	26.13	B
15	ATOM	1902	O	PHE	B	370	42.750	18.584	55.682	1.00	26.19	B
	ATOM	1903	N	VAL	B	371	42.352	17.993	53.556	1.00	25.26	B
	ATOM	1904	CA	VAL	B	371	42.656	16.590	53.811	1.00	24.76	B
	ATOM	1905	CB	VAL	B	371	41.419	15.694	53.697	1.00	25.22	B
	ATOM	1906	CG1	VAL	B	371	41.736	14.297	54.237	1.00	22.91	B
20	ATOM	1907	CG2	VAL	B	371	40.257	16.324	54.442	1.00	23.49	B
	ATOM	1908	C	VAL	B	371	43.712	16.062	52.863	1.00	24.14	B
	ATOM	1909	O	VAL	B	371	43.585	16.188	51.653	1.00	23.89	B
	ATOM	1910	N	PRO	B	372	44.767	15.447	53.418	1.00	24.76	B
	ATOM	1911	CD	PRO	B	372	44.861	15.087	54.840	1.00	25.65	B
25	ATOM	1912	CA	PRO	B	372	45.889	14.878	52.678	1.00	25.57	B
	ATOM	1913	CB	PRO	B	372	46.835	14.390	53.769	1.00	25.32	B
	ATOM	1914	CG	PRO	B	372	46.318	14.998	55.041	1.00	26.54	B
	ATOM	1915	C	PRO	B	372	45.421	13.720	51.863	1.00	27.92	B
	ATOM	1916	O	PRO	B	372	44.359	13.144	52.143	1.00	29.78	B
30	ATOM	1917	N	GLN	B	373	46.223	13.375	50.858	1.00	28.98	B
	ATOM	1918	CA	GLN	B	373	45.940	12.222	50.002	1.00	29.41	B
	ATOM	1919	CB	GLN	B	373	46.566	12.412	48.600	1.00	29.51	B
	ATOM	1920	CG	GLN	B	373	45.660	13.145	47.586	1.00	29.73	B
	ATOM	1921	CD	GLN	B	373	46.354	13.455	46.247	1.00	30.26	B
35	ATOM	1922	OE1	GLN	B	373	47.091	14.429	46.129	1.00	30.70	B
	ATOM	1923	NE2	GLN	B	373	46.113	12.621	45.240	1.00	30.61	B
	ATOM	1924	C	GLN	B	373	46.554	11.029	50.758	1.00	28.67	B
	ATOM	1925	O	GLN	B	373	47.662	11.119	51.274	1.00	28.24	B
	ATOM	1926	N	ARG	B	374	45.803	9.936	50.845	1.00	28.06	B
40	ATOM	1927	CA	ARG	B	374	46.213	8.728	51.557	1.00	25.68	B
	ATOM	1928	CB	ARG	B	374	45.030	8.254	52.416	1.00	25.68	B
	ATOM	1929	CG	ARG	B	374	45.173	6.929	53.159	1.00	24.87	B
	ATOM	1930	CD	ARG	B	374	45.727	7.099	54.544	1.00	25.14	B
	ATOM	1931	NE	ARG	B	374	45.604	5.872	55.347	1.00	26.59	B
45	ATOM	1932	CZ	ARG	B	374	44.549	5.554	56.099	1.00	24.91	B
	ATOM	1933	NH1	ARG	B	374	43.503	6.370	56.171	1.00	23.91	B
	ATOM	1934	NH2	ARG	B	374	44.533	4.407	56.770	1.00	23.39	B
	ATOM	1935	C	ARG	B	374	46.650	7.619	50.598	1.00	25.60	B
	ATOM	1936	O	ARG	B	374	45.978	7.352	49.591	1.00	25.61	B
50	ATOM	1937	N	THR	B	375	47.790	7.000	50.909	1.00	24.83	B
	ATOM	1938	CA	THR	B	375	48.325	5.895	50.124	1.00	24.29	B
	ATOM	1939	CB	THR	B	375	49.562	6.298	49.278	1.00	24.62	B
	ATOM	1940	OG1	THR	B	375	49.334	7.559	48.630	1.00	26.27	B
	ATOM	1941	CG2	THR	B	375	49.845	5.228	48.217	1.00	22.20	B

	ATOM	1942	C	THR	B	375	48.787	4.844	51.125	1.00	25.05	B
	ATOM	1943	O	THR	B	375	49.710	5.108	51.889	1.00	25.56	B
	ATOM	1944	N	THR	B	376	48.149	3.669	51.122	1.00	25.33	B
	ATOM	1945	CA	THR	B	376	48.509	2.571	52.034	1.00	25.61	B
5	ATOM	1946	CB	THR	B	376	47.254	1.951	52.733	1.00	23.00	B
	ATOM	1947	OG1	THR	B	376	46.361	2.992	53.148	1.00	23.90	B
	ATOM	1948	CG2	THR	B	376	47.678	1.125	53.956	1.00	21.63	B
	ATOM	1949	C	THR	B	376	49.224	1.439	51.273	1.00	27.50	B
	ATOM	1950	O	THR	B	376	48.696	0.916	50.303	1.00	27.69	B
10	ATOM	1951	N	LEU	B	377	50.413	1.058	51.735	1.00	29.38	B
	ATOM	1952	CA	LEU	B	377	51.204	-0.001	51.119	1.00	29.82	B
	ATOM	1953	CB	LEU	B	377	52.540	0.574	50.650	1.00	27.89	B
	ATOM	1954	CG	LEU	B	377	52.396	1.871	49.837	1.00	27.64	B
	ATOM	1955	CD1	LEU	B	377	53.754	2.507	49.549	1.00	23.10	B
15	ATOM	1956	CD2	LEU	B	377	51.643	1.570	48.562	1.00	26.07	B
	ATOM	1957	C	LEU	B	377	51.451	-1.131	52.125	1.00	32.73	B
	ATOM	1958	O	LEU	B	377	51.328	-0.925	53.327	1.00	32.89	B
	ATOM	1959	N	ARG	B	378	51.815	-2.315	51.633	1.00	36.51	B
	ATOM	1960	CA	ARG	B	378	52.071	-3.463	52.498	1.00	39.20	B
20	ATOM	1961	CB	ARG	B	378	52.180	-4.757	51.678	1.00	42.06	B
	ATOM	1962	CG	ARG	B	378	52.510	-6.019	52.506	1.00	45.42	B
	ATOM	1963	CD	ARG	B	378	52.472	-7.335	51.682	1.00	48.17	B
	ATOM	1964	NE	ARG	B	378	51.210	-7.513	50.958	1.00	51.30	B
	ATOM	1965	CZ	ARG	B	378	50.850	-8.616	50.306	1.00	52.70	B
25	ATOM	1966	NH1	ARG	B	378	51.655	-9.673	50.281	1.00	53.25	B
	ATOM	1967	NH2	ARG	B	378	49.684	-8.654	49.664	1.00	54.26	B
	ATOM	1968	C	ARG	B	378	53.333	-3.278	53.307	1.00	40.74	B
	ATOM	1969	O	ARG	B	378	54.339	-2.747	52.819	1.00	40.15	B
	ATOM	1970	N	GLY	B	379	53.266	-3.735	54.555	1.00	42.99	B
30	ATOM	1971	CA	GLY	B	379	54.394	-3.628	55.463	1.00	43.31	B
	ATOM	1972	C	GLY	B	379	55.221	-4.897	55.532	1.00	43.80	B
	ATOM	1973	O	GLY	B	379	55.501	-5.532	54.516	1.00	42.41	B
	ATOM	1974	N	HIS	B	380	55.609	-5.264	56.747	1.00	44.62	B
	ATOM	1975	CA	HIS	B	380	56.421	-6.451	56.972	1.00	45.57	B
35	ATOM	1976	CB	HIS	B	380	57.468	-6.163	58.049	1.00	42.95	B
	ATOM	1977	CG	HIS	B	380	58.489	-5.148	57.640	1.00	41.43	B
	ATOM	1978	CD2	HIS	B	380	58.369	-3.842	57.307	1.00	39.61	B
	ATOM	1979	ND1	HIS	B	380	59.833	-5.444	57.559	1.00	40.42	B
	ATOM	1980	CE1	HIS	B	380	60.497	-4.362	57.195	1.00	39.52	B
40	ATOM	1981	NE2	HIS	B	380	59.633	-3.376	57.037	1.00	39.67	B
	ATOM	1982	C	HIS	B	380	55.552	-7.627	57.398	1.00	47.13	B
	ATOM	1983	O	HIS	B	380	54.374	-7.457	57.690	1.00	47.01	B
	ATOM	1984	N	MSE	B	381	56.127	-8.822	57.440	1.00	49.63	B
	ATOM	1985	CA	MSE	B	381	55.350	-9.979	57.826	1.00	51.34	B
45	ATOM	1986	CB	MSE	B	381	56.181	-11.238	57.658	1.00	54.42	B
	ATOM	1987	CG	MSE	B	381	56.131	-11.740	56.225	1.00	60.08	B
	ATOM	1988	SE	MSE	B	381	57.583	-12.923	55.737	1.00	69.56	B
	ATOM	1989	CE	MSE	B	381	56.901	-14.517	56.629	1.00	64.33	B
	ATOM	1990	C	MSE	B	381	54.800	-9.860	59.227	1.00	51.47	B
50	ATOM	1991	O	MSE	B	381	53.645	-10.193	59.464	1.00	53.52	B
	ATOM	1992	N	THR	B	382	55.608	-9.366	60.158	1.00	50.41	B
	ATOM	1993	CA	THR	B	382	55.159	-9.204	61.539	1.00	48.29	B
	ATOM	1994	CB	THR	B	382	56.367	-9.222	62.513	1.00	48.92	B
	ATOM	1995	OG1	THR	B	382	55.931	-8.858	63.825	1.00	49.73	B

	ATOM	1996	CG2	THR	B	382	57.457	-8.259	62.048	1.00	51.19	B
	ATOM	1997	C	THR	B	382	54.361	-7.903	61.674	1.00	46.73	B
	ATOM	1998	O	THR	B	382	54.511	-6.990	60.858	1.00	45.72	B
	ATOM	1999	N	SER	B	383	53.510	-7.818	62.695	1.00	45.75	B
5	ATOM	2000	CA	SER	B	383	52.667	-6.631	62.888	1.00	44.00	B
	ATOM	2001	CB	SER	B	383	51.418	-6.988	63.706	1.00	44.17	B
	ATOM	2002	OG	SER	B	383	51.707	-6.998	65.093	1.00	44.67	B
	ATOM	2003	C	SER	B	383	53.363	-5.440	63.552	1.00	42.52	B
	ATOM	2004	O	SER	B	383	52.739	-4.400	63.769	1.00	42.16	B
10	ATOM	2005	N	VAL	B	384	54.645	-5.584	63.875	1.00	40.61	B
	ATOM	2006	CA	VAL	B	384	55.368	-4.496	64.519	1.00	38.88	B
	ATOM	2007	CB	VAL	B	384	55.785	-4.868	65.971	1.00	37.56	B
	ATOM	2008	CG1	VAL	B	384	56.490	-3.706	66.635	1.00	34.97	B
	ATOM	2009	CG2	VAL	B	384	54.570	-5.273	66.772	1.00	37.83	B
15	ATOM	2010	C	VAL	B	384	56.617	-4.090	63.756	1.00	38.38	B
	ATOM	2011	O	VAL	B	384	57.507	-4.906	63.506	1.00	38.18	B
	ATOM	2012	N	ILE	B	385	56.674	-2.823	63.372	1.00	37.92	B
	ATOM	2013	CA	ILE	B	385	57.842	-2.330	62.674	1.00	38.47	B
	ATOM	2014	CB	ILE	B	385	57.462	-1.284	61.570	1.00	38.37	B
20	ATOM	2015	CG2	ILE	B	385	58.692	-0.795	60.853	1.00	35.43	B
	ATOM	2016	CG1	ILE	B	385	56.610	-1.951	60.483	1.00	38.29	B
	ATOM	2017	CD1	ILE	B	385	56.296	-1.048	59.293	1.00	40.13	B
	ATOM	2018	C	ILE	B	385	58.752	-1.744	63.758	1.00	38.62	B
	ATOM	2019	O	ILE	B	385	58.295	-1.054	64.679	1.00	39.76	B
25	ATOM	2020	N	THR	B	386	60.040	-2.057	63.649	1.00	37.77	B
	ATOM	2021	CA	THR	B	386	61.053	-1.643	64.616	1.00	34.37	B
	ATOM	2022	CB	THR	B	386	62.142	-2.722	64.734	1.00	32.81	B
	ATOM	2023	OG1	THR	B	386	62.810	-2.855	63.473	1.00	31.89	B
	ATOM	2024	CG2	THR	B	386	61.528	-4.050	65.098	1.00	32.45	B
30	ATOM	2025	C	THR	B	386	61.740	-0.329	64.281	1.00	32.70	B
	ATOM	2026	O	THR	B	386	62.088	0.438	65.167	1.00	33.06	B
	ATOM	2027	N	CYS	B	387	61.947	-0.058	63.005	1.00	31.07	B
	ATOM	2028	CA	CYS	B	387	62.627	1.178	62.659	1.00	30.70	B
	ATOM	2029	CB	CYS	B	387	64.140	0.964	62.769	1.00	29.49	B
35	ATOM	2030	SG	CYS	B	387	64.707	-0.568	62.008	1.00	32.59	B
	ATOM	2031	C	CYS	B	387	62.250	1.702	61.268	1.00	29.94	B
	ATOM	2032	O	CYS	B	387	61.896	0.927	60.365	1.00	27.25	B
	ATOM	2033	N	LEU	B	388	62.349	3.021	61.097	1.00	29.32	B
	ATOM	2034	CA	LEU	B	388	62.001	3.659	59.828	1.00	28.34	B
40	ATOM	2035	CB	LEU	B	388	60.534	4.097	59.878	1.00	28.15	B
	ATOM	2036	CG	LEU	B	388	59.848	4.716	58.662	1.00	25.84	B
	ATOM	2037	CD1	LEU	B	388	58.358	4.729	58.925	1.00	26.04	B
	ATOM	2038	CD2	LEU	B	388	60.361	6.117	58.401	1.00	24.86	B
	ATOM	2039	C	LEU	B	388	62.885	4.851	59.479	1.00	26.75	B
45	ATOM	2040	O	LEU	B	388	63.211	5.661	60.336	1.00	25.66	B
	ATOM	2041	N	GLN	B	389	63.284	4.947	58.214	1.00	27.43	B
	ATOM	2042	CA	GLN	B	389	64.112	6.067	57.753	1.00	27.85	B
	ATOM	2043	CB	GLN	B	389	65.505	5.589	57.308	1.00	28.80	B
	ATOM	2044	CG	GLN	B	389	66.450	5.215	58.443	1.00	29.07	B
50	ATOM	2045	CD	GLN	B	389	66.900	6.425	59.249	1.00	29.82	B
	ATOM	2046	OE1	GLN	B	389	67.815	7.152	58.849	1.00	30.35	B
	ATOM	2047	NE2	GLN	B	389	66.244	6.654	60.383	1.00	27.50	B
	ATOM	2048	C	GLN	B	389	63.417	6.718	56.577	1.00	26.75	B
	ATOM	2049	O	GLN	B	389	62.792	6.035	55.766	1.00	26.92	B

	ATOM	2050	N	PHE	B	390	63.532	8.037	56.483	1.00	26.42	B
	ATOM	2051	CA	PHE	B	390	62.928	8.778	55.382	1.00	26.53	B
	ATOM	2052	CB	PHE	B	390	61.606	9.405	55.833	1.00	24.52	B
	ATOM	2053	CG	PHE	B	390	60.846	10.069	54.728	1.00	23.83	B
5	ATOM	2054	CD1	PHE	B	390	60.614	9.408	53.530	1.00	24.31	B
	ATOM	2055	CD2	PHE	B	390	60.357	11.358	54.883	1.00	24.82	B
	ATOM	2056	CE1	PHE	B	390	59.906	10.021	52.496	1.00	24.43	B
	ATOM	2057	CE2	PHE	B	390	59.643	11.985	53.851	1.00	26.18	B
	ATOM	2058	CZ	PHE	B	390	59.418	11.316	52.657	1.00	25.05	B
10	ATOM	2059	C	PHE	B	390	63.885	9.852	54.853	1.00	28.00	B
	ATOM	2060	O	PHE	B	390	64.003	10.930	55.439	1.00	26.52	B
	ATOM	2061	N	GLU	B	391	64.591	9.532	53.761	1.00	31.44	B
	ATOM	2062	CA	GLU	B	391	65.552	10.459	53.112	1.00	34.19	B
	ATOM	2063	CB	GLU	B	391	66.958	10.374	53.753	1.00	35.50	B
15	ATOM	2064	CG	GLU	B	391	67.082	9.731	55.143	1.00	38.57	B
	ATOM	2065	CD	GLU	B	391	66.652	10.654	56.306	1.00	40.82	B
	ATOM	2066	OE1	GLU	B	391	66.842	11.896	56.199	1.00	38.26	B
	ATOM	2067	OE2	GLU	B	391	66.138	10.116	57.327	1.00	41.64	B
	ATOM	2068	C	GLU	B	391	65.706	10.165	51.602	1.00	34.30	B
20	ATOM	2069	O	GLU	B	391	65.415	9.060	51.141	1.00	32.53	B
	ATOM	2070	N	ASP	B	392	66.179	11.151	50.842	1.00	35.27	B
	ATOM	2071	CA	ASP	B	392	66.388	10.979	49.395	1.00	35.87	B
	ATOM	2072	CB	ASP	B	392	67.633	10.114	49.106	1.00	35.92	B
	ATOM	2073	CG	ASP	B	392	68.941	10.886	49.139	1.00	36.64	B
25	ATOM	2074	OD1	ASP	B	392	68.967	12.093	48.795	1.00	37.84	B
	ATOM	2075	OD2	ASP	B	392	69.964	10.253	49.492	1.00	36.21	B
	ATOM	2076	C	ASP	B	392	65.215	10.300	48.673	1.00	36.11	B
	ATOM	2077	O	ASP	B	392	65.452	9.465	47.805	1.00	36.71	B
	ATOM	2078	N	ASN	B	393	63.968	10.618	49.018	1.00	35.71	B
30	ATOM	2079	CA	ASN	B	393	62.805	9.999	48.347	1.00	35.51	B
	ATOM	2080	CB	ASN	B	393	62.861	10.281	46.847	1.00	34.88	B
	ATOM	2081	CG	ASN	B	393	62.762	11.755	46.544	1.00	37.09	B
	ATOM	2082	OD1	ASN	B	393	61.672	12.328	46.584	1.00	36.85	B
	ATOM	2083	ND2	ASN	B	393	63.903	12.388	46.255	1.00	37.57	B
35	ATOM	2084	C	ASN	B	393	62.633	8.489	48.570	1.00	35.26	B
	ATOM	2085	O	ASN	B	393	61.925	7.805	47.817	1.00	34.05	B
	ATOM	2086	N	TYR	B	394	63.283	7.990	49.618	1.00	35.44	B
	ATOM	2087	CA	TYR	B	394	63.246	6.585	50.004	1.00	33.92	B
	ATOM	2088	CB	TYR	B	394	64.660	6.006	50.087	1.00	34.53	B
40	ATOM	2089	CG	TYR	B	394	65.314	5.705	48.772	1.00	35.08	B
	ATOM	2090	CD1	TYR	B	394	64.808	4.707	47.944	1.00	33.82	B
	ATOM	2091	CE1	TYR	B	394	65.424	4.394	46.753	1.00	35.67	B
	ATOM	2092	CD2	TYR	B	394	66.461	6.393	48.370	1.00	33.92	B
	ATOM	2093	CE2	TYR	B	394	67.093	6.091	47.179	1.00	36.23	B
45	ATOM	2094	CZ	TYR	B	394	66.571	5.090	46.369	1.00	37.49	B
	ATOM	2095	OH	TYR	B	394	67.184	4.785	45.167	1.00	39.46	B
	ATOM	2096	C	TYR	B	394	62.652	6.473	51.393	1.00	33.94	B
	ATOM	2097	O	TYR	B	394	62.973	7.268	52.281	1.00	32.72	B
	ATOM	2098	N	VAL	B	395	61.804	5.470	51.575	1.00	33.59	B
50	ATOM	2099	CA	VAL	B	395	61.200	5.196	52.864	1.00	33.27	B
	ATOM	2100	CB	VAL	B	395	59.655	5.170	52.787	1.00	33.84	B
	ATOM	2101	CG1	VAL	B	395	59.055	4.927	54.167	1.00	32.25	B
	ATOM	2102	CG2	VAL	B	395	59.145	6.467	52.213	1.00	34.69	B
	ATOM	2103	C	VAL	B	395	61.708	3.803	53.182	1.00	33.68	B

	ATOM	2104	O	VAL	B	395	61.334	2.822	52.526	1.00	35.51	B
	ATOM	2105	N	ILE	B	396	62.592	3.701	54.163	1.00	33.52	B
	ATOM	2106	CA	ILE	B	396	63.113	2.386	54.508	1.00	32.85	B
	ATOM	2107	CB	ILE	B	396	64.666	2.403	54.579	1.00	33.18	B
5	ATOM	2108	CG2	ILE	B	396	65.207	0.998	54.438	1.00	32.95	B
	ATOM	2109	CG1	ILE	B	396	65.238	3.231	53.434	1.00	32.57	B
	ATOM	2110	CD1	ILE	B	396	66.704	3.519	53.594	1.00	34.98	B
	ATOM	2111	C	ILE	B	396	62.527	1.999	55.862	1.00	30.96	B
	ATOM	2112	O	ILE	B	396	62.550	2.787	56.805	1.00	29.47	B
10	ATOM	2113	N	THR	B	397	61.977	0.792	55.943	1.00	29.81	B
	ATOM	2114	CA	THR	B	397	61.397	0.303	57.188	1.00	30.52	B
	ATOM	2115	CB	THR	B	397	59.883	0.014	57.087	1.00	28.68	B
	ATOM	2116	OG1	THR	B	397	59.685	-1.096	56.216	1.00	27.52	B
	ATOM	2117	CG2	THR	B	397	59.127	1.206	56.561	1.00	28.88	B
15	ATOM	2118	C	THR	B	397	62.052	-1.012	57.574	1.00	32.66	B
	ATOM	2119	O	THR	B	397	62.495	-1.768	56.708	1.00	32.93	B
	ATOM	2120	N	GLY	B	398	62.095	-1.283	58.878	1.00	34.04	B
	ATOM	2121	CA	GLY	B	398	62.673	-2.521	59.377	1.00	36.31	B
	ATOM	2122	C	GLY	B	398	61.790	-3.205	60.409	1.00	38.57	B
20	ATOM	2123	O	GLY	B	398	61.203	-2.535	61.257	1.00	38.84	B
	ATOM	2124	N	ALA	B	399	61.692	-4.532	60.347	1.00	40.48	B
	ATOM	2125	CA	ALA	B	399	60.870	-5.274	61.304	1.00	43.09	B
	ATOM	2126	CB	ALA	B	399	59.540	-5.687	60.660	1.00	43.54	B
	ATOM	2127	C	ALA	B	399	61.577	-6.506	61.870	1.00	44.04	B
25	ATOM	2128	O	ALA	B	399	62.688	-6.838	61.461	1.00	43.75	B
	ATOM	2129	N	ASP	B	400	60.921	-7.182	62.811	1.00	45.72	B
	ATOM	2130	CA	ASP	B	400	61.498	-8.363	63.446	1.00	47.39	B
	ATOM	2131	CB	ASP	B	400	60.854	-8.596	64.820	1.00	48.07	B
	ATOM	2132	CG	ASP	B	400	61.569	-9.666	65.626	1.00	48.91	B
30	ATOM	2133	OD1	ASP	B	400	62.791	-9.515	65.869	1.00	49.38	B
	ATOM	2134	OD2	ASP	B	400	60.910	-10.656	66.012	1.00	48.62	B
	ATOM	2135	C	ASP	B	400	61.347	-9.610	62.579	1.00	47.48	B
	ATOM	2136	O	ASP	B	400	61.522	-10.735	63.048	1.00	49.06	B
	ATOM	2137	N	ASP	B	401	61.014	-9.403	61.313	1.00	46.02	B
35	ATOM	2138	CA	ASP	B	401	60.851	-10.501	60.378	1.00	43.80	B
	ATOM	2139	CB	ASP	B	401	59.688	-10.192	59.436	1.00	45.11	B
	ATOM	2140	CG	ASP	B	401	59.962	-8.996	58.541	1.00	46.35	B
	ATOM	2141	OD1	ASP	B	401	60.797	-8.130	58.909	1.00	46.25	B
	ATOM	2142	OD2	ASP	B	401	59.325	-8.919	57.465	1.00	47.47	B
40	ATOM	2143	C	ASP	B	401	62.147	-10.661	59.592	1.00	42.18	B
	ATOM	2144	O	ASP	B	401	62.153	-11.209	58.498	1.00	40.84	B
	ATOM	2145	N	LYS	B	402	63.241	-10.171	60.174	1.00	42.03	B
	ATOM	2146	CA	LYS	B	402	64.581	-10.221	59.577	1.00	41.37	B
	ATOM	2147	CB	LYS	B	402	65.061	-11.671	59.394	1.00	41.89	B
45	ATOM	2148	CG	LYS	B	402	64.777	-12.595	60.546	1.00	40.16	B
	ATOM	2149	CD	LYS	B	402	65.248	-14.004	60.249	1.00	39.21	B
	ATOM	2150	CE	LYS	B	402	64.973	-14.910	61.453	1.00	41.18	B
	ATOM	2151	NZ	LYS	B	402	65.506	-16.306	61.313	1.00	41.31	B
	ATOM	2152	C	LYS	B	402	64.584	-9.545	58.217	1.00	41.18	B
50	ATOM	2153	O	LYS	B	402	65.387	-9.880	57.350	1.00	41.03	B
	ATOM	2154	N	MSE	B	403	63.700	-8.583	58.021	1.00	41.52	B
	ATOM	2155	CA	MSE	B	403	63.643	-7.932	56.731	1.00	41.52	B
	ATOM	2156	CB	MSE	B	403	62.364	-8.354	56.024	1.00	44.20	B
	ATOM	2157	CG	MSE	B	403	62.593	-8.927	54.649	1.00	49.51	B

	ATOM	2158	SE	MSE	B	403	63.401	-10.704	54.630	1.00	56.96	B
	ATOM	2159	CE	MSE	B	403	61.754	-11.724	54.910	1.00	52.63	B
	ATOM	2160	C	MSE	B	403	63.728	-6.408	56.765	1.00	39.82	B
	ATOM	2161	O	MSE	B	403	63.396	-5.758	57.763	1.00	39.40	B
5	ATOM	2162	N	ILE	B	404	64.163	-5.861	55.638	1.00	37.19	B
	ATOM	2163	CA	ILE	B	404	64.305	-4.432	55.441	1.00	34.55	B
	ATOM	2164	CB	ILE	B	404	65.790	-4.049	55.290	1.00	33.79	B
	ATOM	2165	CG2	ILE	B	404	65.904	-2.619	54.750	1.00	32.01	B
	ATOM	2166	CG1	ILE	B	404	66.516	-4.256	56.628	1.00	32.98	B
10	ATOM	2167	CD1	ILE	B	404	68.003	-3.868	56.634	1.00	32.54	B
	ATOM	2168	C	ILE	B	404	63.576	-4.060	54.152	1.00	34.51	B
	ATOM	2169	O	ILE	B	404	63.994	-4.455	53.061	1.00	33.17	B
	ATOM	2170	N	ARG	B	405	62.489	-3.303	54.275	1.00	34.07	B
	ATOM	2171	CA	ARG	B	405	61.714	-2.890	53.104	1.00	34.11	B
15	ATOM	2172	CB	ARG	B	405	60.222	-3.145	53.349	1.00	31.76	B
	ATOM	2173	CG	ARG	B	405	59.877	-4.612	53.569	1.00	29.64	B
	ATOM	2174	CD	ARG	B	405	58.419	-4.820	53.979	1.00	28.14	B
	ATOM	2175	NE	ARG	B	405	57.449	-4.457	52.948	1.00	28.57	B
	ATOM	2176	CZ	ARG	B	405	57.252	-5.129	51.813	1.00	28.90	B
20	ATOM	2177	NH1	ARG	B	405	57.964	-6.215	51.537	1.00	25.04	B
	ATOM	2178	NH2	ARG	B	405	56.311	-4.728	50.960	1.00	29.02	B
	ATOM	2179	C	ARG	B	405	61.912	-1.425	52.730	1.00	34.97	B
	ATOM	2180	O	ARG	B	405	61.823	-0.545	53.580	1.00	37.29	B
	ATOM	2181	N	VAL	B	406	62.180	-1.157	51.460	1.00	34.65	B
25	ATOM	2182	CA	VAL	B	406	62.353	0.218	51.027	1.00	35.39	B
	ATOM	2183	CB	VAL	B	406	63.710	0.421	50.341	1.00	38.27	B
	ATOM	2184	CG1	VAL	B	406	63.886	-0.606	49.251	1.00	39.50	B
	ATOM	2185	CG2	VAL	B	406	63.789	1.831	49.759	1.00	38.99	B
	ATOM	2186	C	VAL	B	406	61.257	0.576	50.041	1.00	34.13	B
30	ATOM	2187	O	VAL	B	406	60.867	-0.250	49.213	1.00	35.33	B
	ATOM	2188	N	TYR	B	407	60.763	1.806	50.127	1.00	32.42	B
	ATOM	2189	CA	TYR	B	407	59.694	2.263	49.236	1.00	30.87	B
	ATOM	2190	CB	TYR	B	407	58.409	2.537	50.032	1.00	30.46	B
	ATOM	2191	CG	TYR	B	407	57.953	1.435	50.967	1.00	29.77	B
35	ATOM	2192	CD1	TYR	B	407	58.682	1.115	52.121	1.00	27.81	B
	ATOM	2193	CE1	TYR	B	407	58.269	0.081	52.962	1.00	27.20	B
	ATOM	2194	CD2	TYR	B	407	56.795	0.695	50.682	1.00	29.18	B
	ATOM	2195	CE2	TYR	B	407	56.376	-0.335	51.511	1.00	27.89	B
	ATOM	2196	CZ	TYR	B	407	57.114	-0.645	52.646	1.00	27.80	B
40	ATOM	2197	OH	TYR	B	407	56.711	-1.705	53.430	1.00	26.41	B
	ATOM	2198	C	TYR	B	407	60.058	3.552	48.507	1.00	29.93	B
	ATOM	2199	O	TYR	B	407	61.078	4.180	48.790	1.00	30.68	B
	ATOM	2200	N	ASP	B	408	59.189	3.947	47.583	1.00	29.96	B
	ATOM	2201	CA	ASP	B	408	59.360	5.181	46.825	1.00	30.52	B
45	ATOM	2202	CB	ASP	B	408	59.226	4.920	45.325	1.00	32.17	B
	ATOM	2203	CG	ASP	B	408	59.430	6.178	44.504	1.00	35.42	B
	ATOM	2204	OD1	ASP	B	408	60.450	6.868	44.721	1.00	37.74	B
	ATOM	2205	OD2	ASP	B	408	58.579	6.483	43.644	1.00	37.68	B
	ATOM	2206	C	ASP	B	408	58.296	6.195	47.264	1.00	29.92	B
50	ATOM	2207	O	ASP	B	408	57.095	5.995	47.024	1.00	29.81	B
	ATOM	2208	N	SER	B	409	58.743	7.284	47.895	1.00	28.80	B
	ATOM	2209	CA	SER	B	409	57.848	8.338	48.400	1.00	28.18	B
	ATOM	2210	CB	SER	B	409	58.581	9.202	49.442	1.00	25.85	B
	ATOM	2211	OG	SER	B	409	59.652	9.932	48.869	1.00	23.45	B

	ATOM	2212	C	SER	B	409	57.253	9.245	47.320	1.00	29.34	B
	ATOM	2213	O	SER	B	409	56.259	9.941	47.562	1.00	27.47	B
	ATOM	2214	N	ILE	B	410	57.861	9.224	46.133	1.00	31.65	B
	ATOM	2215	CA	ILE	B	410	57.421	10.037	44.994	1.00	34.03	B
5	ATOM	2216	CB	ILE	B	410	58.558	10.242	43.972	1.00	35.56	B
	ATOM	2217	CG2	ILE	B	410	58.032	11.052	42.783	1.00	34.67	B
	ATOM	2218	CG1	ILE	B	410	59.747	10.947	44.616	1.00	34.10	B
	ATOM	2219	CD1	ILE	B	410	60.988	10.910	43.752	1.00	33.88	B
	ATOM	2220	C	ILE	B	410	56.259	9.409	44.217	1.00	34.05	B
10	ATOM	2221	O	ILE	B	410	55.330	10.101	43.818	1.00	33.24	B
	ATOM	2222	N	ASN	B	411	56.354	8.107	43.972	1.00	34.44	B
	ATOM	2223	CA	ASN	B	411	55.327	7.390	43.246	1.00	36.84	B
	ATOM	2224	CB	ASN	B	411	55.955	6.377	42.273	1.00	39.14	B
	ATOM	2225	CG	ASN	B	411	56.312	6.993	40.911	1.00	41.27	B
15	ATOM	2226	OD1	ASN	B	411	56.852	8.100	40.834	1.00	41.10	B
	ATOM	2227	ND2	ASN	B	411	56.017	6.261	39.832	1.00	42.48	B
	ATOM	2228	C	ASN	B	411	54.428	6.663	44.238	1.00	37.14	B
	ATOM	2229	O	ASN	B	411	53.466	6.001	43.848	1.00	37.86	B
	ATOM	2230	N	LYS	B	412	54.748	6.776	45.522	1.00	36.65	B
20	ATOM	2231	CA	LYS	B	412	53.944	6.121	46.546	1.00	35.90	B
	ATOM	2232	CB	LYS	B	412	52.537	6.742	46.595	1.00	35.46	B
	ATOM	2233	CG	LYS	B	412	52.373	7.994	47.470	1.00	34.91	B
	ATOM	2234	CD	LYS	B	412	53.251	9.163	47.023	1.00	33.80	B
	ATOM	2235	CE	LYS	B	412	52.905	10.407	47.809	1.00	32.17	B
25	ATOM	2236	NZ	LYS	B	412	53.762	11.553	47.463	1.00	32.35	B
	ATOM	2237	C	LYS	B	412	53.812	4.629	46.256	1.00	35.57	B
	ATOM	2238	O	LYS	B	412	52.703	4.092	46.252	1.00	35.07	B
	ATOM	2239	N	LYS	B	413	54.932	3.959	46.007	1.00	35.95	B
	ATOM	2240	CA	LYS	B	413	54.901	2.523	45.721	1.00	36.16	B
30	ATOM	2241	CB	LYS	B	413	54.977	2.254	44.205	1.00	36.93	B
	ATOM	2242	CG	LYS	B	413	53.730	2.627	43.387	1.00	40.07	B
	ATOM	2243	CD	LYS	B	413	53.913	2.308	41.900	1.00	41.03	B
	ATOM	2244	CE	LYS	B	413	52.629	2.529	41.105	1.00	42.27	B
	ATOM	2245	NZ	LYS	B	413	51.504	1.699	41.610	1.00	43.62	B
35	ATOM	2246	C	LYS	B	413	56.047	1.798	46.402	1.00	35.81	B
	ATOM	2247	O	LYS	B	413	57.012	2.417	46.841	1.00	33.26	B
	ATOM	2248	N	PHE	B	414	55.904	0.481	46.503	1.00	38.03	B
	ATOM	2249	CA	PHE	B	414	56.909	-0.402	47.090	1.00	39.76	B
	ATOM	2250	CB	PHE	B	414	56.267	-1.749	47.454	1.00	40.36	B
40	ATOM	2251	CG	PHE	B	414	57.257	-2.806	47.872	1.00	42.43	B
	ATOM	2252	CD1	PHE	B	414	57.994	-2.667	49.046	1.00	43.87	B
	ATOM	2253	CD2	PHE	B	414	57.499	-3.914	47.058	1.00	41.81	B
	ATOM	2254	CE1	PHE	B	414	58.965	-3.614	49.398	1.00	43.95	B
	ATOM	2255	CE2	PHE	B	414	58.466	-4.863	47.401	1.00	41.35	B
45	ATOM	2256	CZ	PHE	B	414	59.201	-4.712	48.571	1.00	42.36	B
	ATOM	2257	C	PHE	B	414	57.970	-0.598	46.003	1.00	40.17	B
	ATOM	2258	O	PHE	B	414	57.642	-0.894	44.854	1.00	39.12	B
	ATOM	2259	N	LEU	B	415	59.236	-0.425	46.361	1.00	41.37	B
	ATOM	2260	CA	LEU	B	415	60.305	-0.558	45.386	1.00	42.80	B
50	ATOM	2261	CB	LEU	B	415	61.350	0.539	45.608	1.00	44.70	B
	ATOM	2262	CG	LEU	B	415	62.211	0.891	44.391	1.00	46.65	B
	ATOM	2263	CD1	LEU	B	415	61.335	1.453	43.273	1.00	46.10	B
	ATOM	2264	CD2	LEU	B	415	63.277	1.905	44.794	1.00	47.87	B
	ATOM	2265	C	LEU	B	415	60.950	-1.941	45.464	1.00	43.04	B

	ATOM	2266	O	LEU	B	415	60.930	-2.699	44.503	1.00	42.67	B
	ATOM	2267	N	LEU	B	416	61.531	-2.288	46.600	1.00	43.99	B
	ATOM	2268	CA	LEU	B	416	62.140	-3.607	46.711	1.00	44.67	B
	ATOM	2269	CB	LEU	B	416	63.471	-3.667	45.948	1.00	43.56	B
5	ATOM	2270	CG	LEU	B	416	64.709	-3.198	46.703	1.00	42.12	B
	ATOM	2271	CD1	LEU	B	416	65.621	-4.380	46.873	1.00	45.95	B
	ATOM	2272	CD2	LEU	B	416	65.421	-2.101	45.951	1.00	41.53	B
	ATOM	2273	C	LEU	B	416	62.363	-3.960	48.165	1.00	44.94	B
	ATOM	2274	O	LEU	B	416	62.183	-3.123	49.060	1.00	45.50	B
10	ATOM	2275	N	GLN	B	417	62.747	-5.212	48.393	1.00	45.21	B
	ATOM	2276	CA	GLN	B	417	62.999	-5.712	49.744	1.00	45.08	B
	ATOM	2277	CB	GLN	B	417	61.984	-6.808	50.120	1.00	43.81	B
	ATOM	2278	CG	GLN	B	417	62.106	-7.321	51.555	1.00	40.41	B
	ATOM	2279	CD	GLN	B	417	61.077	-8.383	51.890	1.00	39.74	B
15	ATOM	2280	OE1	GLN	B	417	61.135	-9.507	51.390	1.00	41.92	B
	ATOM	2281	NE2	GLN	B	417	60.129	-8.033	52.741	1.00	38.39	B
	ATOM	2282	C	GLN	B	417	64.412	-6.279	49.844	1.00	44.86	B
	ATOM	2283	O	GLN	B	417	64.906	-6.895	48.897	1.00	43.18	B
	ATOM	2284	N	LEU	B	418	65.053	-6.053	50.991	1.00	45.20	B
20	ATOM	2285	CA	LEU	B	418	66.408	-6.536	51.246	1.00	44.82	B
	ATOM	2286	CB	LEU	B	418	67.329	-5.373	51.654	1.00	42.07	B
	ATOM	2287	CG	LEU	B	418	67.665	-4.358	50.550	1.00	40.04	B
	ATOM	2288	CD1	LEU	B	418	67.984	-2.989	51.123	1.00	38.25	B
	ATOM	2289	CD2	LEU	B	418	68.804	-4.885	49.746	1.00	39.20	B
25	ATOM	2290	C	LEU	B	418	66.337	-7.584	52.357	1.00	46.53	B
	ATOM	2291	O	LEU	B	418	65.728	-7.355	53.411	1.00	46.91	B
	ATOM	2292	N	SER	B	419	66.929	-8.747	52.086	1.00	47.50	B
	ATOM	2293	CA	SER	B	419	66.966	-9.854	53.037	1.00	47.26	B
	ATOM	2294	CB	SER	B	419	66.219	-11.066	52.489	1.00	47.58	B
30	ATOM	2295	OG	SER	B	419	66.861	-11.552	51.330	1.00	47.48	B
	ATOM	2296	C	SER	B	419	68.423	-10.219	53.282	1.00	47.06	B
	ATOM	2297	O	SER	B	419	69.267	-10.064	52.396	1.00	46.04	B
	ATOM	2298	N	GLY	B	420	68.700	-10.697	54.493	1.00	47.22	B
	ATOM	2299	CA	GLY	B	420	70.047	-11.059	54.886	1.00	46.53	B
35	ATOM	2300	C	GLY	B	420	70.121	-11.386	56.366	1.00	47.16	B
	ATOM	2301	O	GLY	B	420	70.335	-12.546	56.715	1.00	48.39	B
	ATOM	2302	N	HIS	B	421	69.927	-10.390	57.237	1.00	46.12	B
	ATOM	2303	CA	HIS	B	421	69.999	-10.611	58.697	1.00	44.26	B
	ATOM	2304	CB	HIS	B	421	69.340	-9.451	59.469	1.00	42.53	B
40	ATOM	2305	CG	HIS	B	421	70.144	-8.187	59.459	1.00	41.48	B
	ATOM	2306	CD2	HIS	B	421	70.083	-7.102	58.653	1.00	41.32	B
	ATOM	2307	ND1	HIS	B	421	71.231	-7.991	60.282	1.00	41.41	B
	ATOM	2308	CE1	HIS	B	421	71.811	-6.845	59.977	1.00	41.09	B
	ATOM	2309	NE2	HIS	B	421	71.135	-6.286	58.990	1.00	40.64	B
45	ATOM	2310	C	HIS	B	421	69.374	-11.937	59.142	1.00	44.07	B
	ATOM	2311	O	HIS	B	421	68.254	-12.277	58.746	1.00	43.02	B
	ATOM	2312	N	ASP	B	422	70.103	-12.687	59.964	1.00	43.55	B
	ATOM	2313	CA	ASP	B	422	69.599	-13.967	60.447	1.00	43.78	B
	ATOM	2314	CB	ASP	B	422	70.752	-14.881	60.881	1.00	46.42	B
50	ATOM	2315	CG	ASP	B	422	71.843	-15.013	59.811	1.00	48.64	B
	ATOM	2316	OD1	ASP	B	422	71.518	-15.368	58.649	1.00	47.48	B
	ATOM	2317	OD2	ASP	B	422	73.030	-14.762	60.145	1.00	50.00	B
	ATOM	2318	C	ASP	B	422	68.634	-13.762	61.609	1.00	42.50	B
	ATOM	2319	O	ASP	B	422	67.970	-14.701	62.048	1.00	41.14	B

	ATOM	2320	N	GLY	B	423	68.561	-12.527	62.099	1.00	42.77	B
	ATOM	2321	CA	GLY	B	423	67.659	-12.192	63.195	1.00	42.60	B
	ATOM	2322	C	GLY	B	423	66.843	-10.950	62.865	1.00	41.88	B
	ATOM	2323	O	GLY	B	423	67.107	-10.300	61.855	1.00	42.25	B
5	ATOM	2324	N	GLY	B	424	65.854	-10.615	63.694	1.00	41.87	B
	ATOM	2325	CA	GLY	B	424	65.036	-9.432	63.433	1.00	41.62	B
	ATOM	2326	C	GLY	B	424	65.863	-8.158	63.492	1.00	41.35	B
	ATOM	2327	O	GLY	B	424	66.673	-7.994	64.389	1.00	41.29	B
	ATOM	2328	N	VAL	B	425	65.682	-7.254	62.541	1.00	41.10	B
10	ATOM	2329	CA	VAL	B	425	66.452	-6.015	62.557	1.00	42.45	B
	ATOM	2330	CB	VAL	B	425	66.622	-5.464	61.137	1.00	44.73	B
	ATOM	2331	CG1	VAL	B	425	65.322	-5.641	60.365	1.00	45.42	B
	ATOM	2332	CG2	VAL	B	425	67.028	-3.987	61.187	1.00	45.68	B
	ATOM	2333	C	VAL	B	425	65.796	-4.946	63.433	1.00	41.72	B
15	ATOM	2334	O	VAL	B	425	64.600	-4.702	63.318	1.00	42.42	B
	ATOM	2335	N	TRP	B	426	66.575	-4.305	64.301	1.00	40.55	B
	ATOM	2336	CA	TRP	B	426	66.016	-3.284	65.177	1.00	39.71	B
	ATOM	2337	CB	TRP	B	426	66.069	-3.755	66.632	1.00	36.69	B
	ATOM	2338	CG	TRP	B	426	65.117	-4.874	66.920	1.00	34.11	B
20	ATOM	2339	CD2	TRP	B	426	63.831	-4.774	67.558	1.00	32.48	B
	ATOM	2340	CE2	TRP	B	426	63.275	-6.072	67.578	1.00	30.88	B
	ATOM	2341	CE3	TRP	B	426	63.098	-3.715	68.110	1.00	30.22	B
	ATOM	2342	CD1	TRP	B	426	65.278	-6.185	66.594	1.00	33.27	B
	ATOM	2343	NE1	TRP	B	426	64.179	-6.910	66.984	1.00	32.30	B
25	ATOM	2344	CZ2	TRP	B	426	62.017	-6.344	68.129	1.00	31.05	B
	ATOM	2345	CZ3	TRP	B	426	61.845	-3.984	68.661	1.00	30.71	B
	ATOM	2346	CH2	TRP	B	426	61.319	-5.289	68.666	1.00	30.24	B
	ATOM	2347	C	TRP	B	426	66.631	-1.889	65.066	1.00	40.31	B
	ATOM	2348	O	TRP	B	426	66.089	-0.930	65.607	1.00	40.76	B
30	ATOM	2349	N	ALA	B	427	67.759	-1.774	64.379	1.00	41.09	B
	ATOM	2350	CA	ALA	B	427	68.400	-0.482	64.198	1.00	42.24	B
	ATOM	2351	CB	ALA	B	427	69.783	-0.481	64.816	1.00	42.58	B
	ATOM	2352	C	ALA	B	427	68.488	-0.284	62.695	1.00	43.39	B
	ATOM	2353	O	ALA	B	427	68.658	-1.251	61.952	1.00	44.01	B
35	ATOM	2354	N	LEU	B	428	68.375	0.963	62.248	1.00	44.59	B
	ATOM	2355	CA	LEU	B	428	68.401	1.261	60.821	1.00	44.89	B
	ATOM	2356	CB	LEU	B	428	67.015	0.996	60.230	1.00	45.56	B
	ATOM	2357	CG	LEU	B	428	66.894	0.895	58.717	1.00	46.48	B
	ATOM	2358	CD1	LEU	B	428	67.730	-0.281	58.221	1.00	47.28	B
40	ATOM	2359	CD2	LEU	B	428	65.434	0.710	58.349	1.00	46.47	B
	ATOM	2360	C	LEU	B	428	68.761	2.714	60.608	1.00	44.99	B
	ATOM	2361	O	LEU	B	428	68.132	3.596	61.178	1.00	46.41	B
	ATOM	2362	N	LYS	B	429	69.766	2.969	59.785	1.00	44.76	B
	ATOM	2363	CA	LYS	B	429	70.189	4.341	59.519	1.00	44.20	B
45	ATOM	2364	CB	LYS	B	429	71.478	4.631	60.288	1.00	43.86	B
	ATOM	2365	CG	LYS	B	429	72.022	6.021	60.108	1.00	43.02	B
	ATOM	2366	CD	LYS	B	429	71.151	7.060	60.779	1.00	40.87	B
	ATOM	2367	CE	LYS	B	429	71.741	8.447	60.560	1.00	38.32	B
	ATOM	2368	NZ	LYS	B	429	71.164	9.464	61.464	1.00	34.95	B
50	ATOM	2369	C	LYS	B	429	70.406	4.457	58.021	1.00	44.44	B
	ATOM	2370	O	LYS	B	429	70.534	3.445	57.344	1.00	44.65	B
	ATOM	2371	N	TYR	B	430	70.430	5.677	57.496	1.00	45.98	B
	ATOM	2372	CA	TYR	B	430	70.617	5.884	56.052	1.00	46.60	B
	ATOM	2373	CB	TYR	B	430	69.403	6.616	55.458	1.00	43.95	B

5	ATOM	2374	CG	TYR	B	430	69.496	6.911	53.973	1.00	41.46	B
	ATOM	2375	CD1	TYR	B	430	69.092	5.976	53.027	1.00	40.19	B
	ATOM	2376	CE1	TYR	B	430	69.153	6.255	51.664	1.00	38.85	B
	ATOM	2377	CD2	TYR	B	430	69.968	8.137	53.520	1.00	40.10	B
	ATOM	2378	CE2	TYR	B	430	70.034	8.430	52.164	1.00	39.82	B
10	ATOM	2379	CZ	TYR	B	430	69.625	7.486	51.232	1.00	39.47	B
	ATOM	2380	OH	TYR	B	430	69.691	7.784	49.874	1.00	37.41	B
	ATOM	2381	C	TYR	B	430	71.872	6.696	55.767	1.00	47.43	B
	ATOM	2382	O	TYR	B	430	72.320	7.476	56.603	1.00	48.99	B
	ATOM	2383	N	ALA	B	431	72.439	6.516	54.582	1.00	48.65	B
15	ATOM	2384	CA	ALA	B	431	73.634	7.263	54.196	1.00	48.95	B
	ATOM	2385	CB	ALA	B	431	74.882	6.412	54.420	1.00	49.04	B
	ATOM	2386	C	ALA	B	431	73.533	7.683	52.732	1.00	49.00	B
	ATOM	2387	O	ALA	B	431	73.298	6.860	51.842	1.00	48.35	B
	ATOM	2388	N	HIS	B	432	73.729	8.967	52.482	1.00	49.81	B
20	ATOM	2389	CA	HIS	B	432	73.627	9.485	51.126	1.00	52.51	B
	ATOM	2390	CB	HIS	B	432	74.421	10.787	50.978	1.00	55.86	B
	ATOM	2391	CG	HIS	B	432	74.148	11.508	49.695	1.00	60.52	B
	ATOM	2392	CD2	HIS	B	432	74.984	12.012	48.757	1.00	62.00	B
	ATOM	2393	ND1	HIS	B	432	72.869	11.750	49.238	1.00	62.73	B
25	ATOM	2394	CE1	HIS	B	432	72.930	12.368	48.072	1.00	63.55	B
	ATOM	2395	NE2	HIS	B	432	74.202	12.539	47.757	1.00	63.41	B
	ATOM	2396	C	HIS	B	432	74.084	8.497	50.059	1.00	51.80	B
	ATOM	2397	O	HIS	B	432	75.031	7.737	50.266	1.00	53.10	B
	ATOM	2398	N	GLY	B	433	73.391	8.508	48.923	1.00	50.58	B
30	ATOM	2399	CA	GLY	B	433	73.741	7.633	47.819	1.00	47.93	B
	ATOM	2400	C	GLY	B	433	72.921	6.368	47.714	1.00	47.35	B
	ATOM	2401	O	GLY	B	433	73.272	5.462	46.963	1.00	47.94	B
	ATOM	2402	N	GLY	B	434	71.823	6.293	48.452	1.00	46.94	B
	ATOM	2403	CA	GLY	B	434	71.016	5.090	48.392	1.00	45.51	B
35	ATOM	2404	C	GLY	B	434	71.722	3.980	49.147	1.00	44.93	B
	ATOM	2405	O	GLY	B	434	71.599	2.804	48.824	1.00	45.17	B
	ATOM	2406	N	ILE	B	435	72.501	4.353	50.151	1.00	44.36	B
	ATOM	2407	CA	ILE	B	435	73.183	3.352	50.943	1.00	43.99	B
	ATOM	2408	CB	ILE	B	435	74.701	3.520	50.874	1.00	43.64	B
40	ATOM	2409	CG2	ILE	B	435	75.375	2.722	51.989	1.00	43.26	B
	ATOM	2410	CG1	ILE	B	435	75.196	3.022	49.528	1.00	43.31	B
	ATOM	2411	CD1	ILE	B	435	76.656	3.223	49.321	1.00	45.00	B
	ATOM	2412	C	ILE	B	435	72.724	3.435	52.395	1.00	44.68	B
	ATOM	2413	O	ILE	B	435	72.570	4.518	52.956	1.00	42.73	B
45	ATOM	2414	N	LEU	B	436	72.486	2.283	53.000	1.00	44.69	B
	ATOM	2415	CA	LEU	B	436	72.051	2.273	54.376	1.00	46.18	B
	ATOM	2416	CB	LEU	B	436	70.545	2.006	54.468	1.00	46.74	B
	ATOM	2417	CG	LEU	B	436	70.020	0.623	54.084	1.00	46.70	B
	ATOM	2418	CD1	LEU	B	436	68.660	0.398	54.708	1.00	47.92	B
50	ATOM	2419	CD2	LEU	B	436	69.953	0.506	52.574	1.00	48.12	B
	ATOM	2420	C	LEU	B	436	72.816	1.224	55.176	1.00	47.09	B
	ATOM	2421	O	LEU	B	436	73.360	0.268	54.619	1.00	46.99	B
	ATOM	2422	N	VAL	B	437	72.862	1.418	56.488	1.00	46.98	B
	ATOM	2423	CA	VAL	B	437	73.552	0.497	57.376	1.00	48.04	B
	ATOM	2424	CB	VAL	B	437	74.617	1.244	58.228	1.00	49.43	B
	ATOM	2425	CG1	VAL	B	437	75.517	0.251	58.948	1.00	48.59	B
	ATOM	2426	CG2	VAL	B	437	75.443	2.180	57.333	1.00	49.25	B
	ATOM	2427	C	VAL	B	437	72.481	-0.062	58.299	1.00	46.89	B

	ATOM	2428	O	VAL	B	437	71.430	0.551	58.449	1.00	47.34	B
	ATOM	2429	N	SER	B	438	72.722	-1.222	58.902	1.00	45.63	B
	ATOM	2430	CA	SER	B	438	71.741	-1.788	59.820	1.00	44.89	B
	ATOM	2431	CB	SER	B	438	70.729	-2.644	59.072	1.00	44.08	B
5	ATOM	2432	OG	SER	B	438	71.355	-3.758	58.467	1.00	44.83	B
	ATOM	2433	C	SER	B	438	72.377	-2.622	60.914	1.00	44.82	B
	ATOM	2434	O	SER	B	438	73.561	-2.949	60.857	1.00	44.21	B
	ATOM	2435	N	GLY	B	439	71.568	-2.945	61.916	1.00	45.02	B
	ATOM	2436	CA	GLY	B	439	72.020	-3.751	63.027	1.00	45.90	B
10	ATOM	2437	C	GLY	B	439	70.855	-4.596	63.498	1.00	46.75	B
	ATOM	2438	O	GLY	B	439	69.809	-4.054	63.843	1.00	45.99	B
	ATOM	2439	N	SER	B	440	71.006	-5.915	63.496	1.00	49.24	B
	ATOM	2440	CA	SER	B	440	69.919	-6.773	63.957	1.00	53.65	B
	ATOM	2441	CB	SER	B	440	69.429	-7.707	62.842	1.00	54.51	B
15	ATOM	2442	OG	SER	B	440	70.342	-8.766	62.610	1.00	56.40	B
	ATOM	2443	C	SER	B	440	70.368	-7.612	65.146	1.00	54.82	B
	ATOM	2444	O	SER	B	440	71.474	-7.447	65.660	1.00	54.64	B
	ATOM	2445	N	THR	B	441	69.490	-8.509	65.576	1.00	57.06	B
	ATOM	2446	CA	THR	B	441	69.769	-9.392	66.695	1.00	59.13	B
20	ATOM	2447	CB	THR	B	441	68.498	-10.086	67.165	1.00	57.43	B
	ATOM	2448	OG1	THR	B	441	67.489	-9.101	67.397	1.00	55.10	B
	ATOM	2449	CG2	THR	B	441	68.761	-10.835	68.455	1.00	59.62	B
	ATOM	2450	C	THR	B	441	70.778	-10.442	66.262	1.00	61.73	B
	ATOM	2451	O	THR	B	441	71.212	-11.280	67.048	1.00	62.25	B
25	ATOM	2452	N	ASP	B	442	71.142	-10.379	64.989	1.00	64.11	B
	ATOM	2453	CA	ASP	B	442	72.098	-11.292	64.403	1.00	65.34	B
	ATOM	2454	CB	ASP	B	442	72.028	-11.183	62.877	1.00	69.79	B
	ATOM	2455	CG	ASP	B	442	72.888	-12.220	62.171	1.00	76.04	B
	ATOM	2456	OD1	ASP	B	442	72.837	-13.413	62.567	1.00	78.67	B
30	ATOM	2457	OD2	ASP	B	442	73.607	-11.846	61.208	1.00	78.25	B
	ATOM	2458	C	ASP	B	442	73.490	-10.929	64.903	1.00	64.29	B
	ATOM	2459	O	ASP	B	442	74.469	-11.621	64.626	1.00	65.24	B
	ATOM	2460	N	ARG	B	443	73.561	-9.843	65.662	1.00	62.52	B
	ATOM	2461	CA	ARG	B	443	74.817	-9.346	66.214	1.00	60.60	B
35	ATOM	2462	CB	ARG	B	443	75.495	-10.412	67.088	1.00	61.78	B
	ATOM	2463	CG	ARG	B	443	74.629	-10.891	68.231	1.00	64.13	B
	ATOM	2464	CD	ARG	B	443	75.329	-11.918	69.100	1.00	65.45	B
	ATOM	2465	NE	ARG	B	443	75.805	-13.045	68.312	1.00	68.14	B
	ATOM	2466	CZ	ARG	B	443	76.062	-14.252	68.804	1.00	69.90	B
40	ATOM	2467	NH1	ARG	B	443	75.885	-14.495	70.096	1.00	69.79	B
	ATOM	2468	NH2	ARG	B	443	76.493	-15.219	67.998	1.00	70.62	B
	ATOM	2469	C	ARG	B	443	75.754	-8.904	65.100	1.00	58.12	B
	ATOM	2470	O	ARG	B	443	76.972	-8.886	65.266	1.00	58.34	B
	ATOM	2471	N	THR	B	444	75.183	-8.534	63.960	1.00	55.54	B
45	ATOM	2472	CA	THR	B	444	76.005	-8.092	62.841	1.00	53.90	B
	ATOM	2473	CB	THR	B	444	75.945	-9.106	61.671	1.00	54.03	B
	ATOM	2474	OG1	THR	B	444	74.590	-9.262	61.232	1.00	53.30	B
	ATOM	2475	CG2	THR	B	444	76.482	-10.464	62.113	1.00	53.83	B
	ATOM	2476	C	THR	B	444	75.567	-6.727	62.338	1.00	51.81	B
50	ATOM	2477	O	THR	B	444	74.401	-6.377	62.409	1.00	52.22	B
	ATOM	2478	N	VAL	B	445	76.510	-5.945	61.846	1.00	49.88	B
	ATOM	2479	CA	VAL	B	445	76.169	-4.641	61.330	1.00	49.27	B
	ATOM	2480	CB	VAL	B	445	77.158	-3.569	61.825	1.00	48.34	B
	ATOM	2481	CG1	VAL	B	445	76.756	-2.196	61.303	1.00	47.11	B

	ATOM	2482	CG2	VAL	B	445	77.192	-3.566	63.349	1.00	48.46	B
	ATOM	2483	C	VAL	B	445	76.233	-4.745	59.813	1.00	50.36	B
	ATOM	2484	O	VAL	B	445	77.308	-4.656	59.209	1.00	50.35	B
	ATOM	2485	N	ARG	B	446	75.080	-4.959	59.194	1.00	50.86	B
5	ATOM	2486	CA	ARG	B	446	75.039	-5.081	57.749	1.00	51.42	B
	ATOM	2487	CB	ARG	B	446	74.024	-6.152	57.329	1.00	52.81	B
	ATOM	2488	CG	ARG	B	446	74.384	-7.595	57.725	1.00	53.32	B
	ATOM	2489	CD	ARG	B	446	73.563	-8.565	56.893	1.00	54.70	B
	ATOM	2490	NE	ARG	B	446	73.801	-9.970	57.206	1.00	55.46	B
10	ATOM	2491	CZ	ARG	B	446	73.462	-10.545	58.353	1.00	57.14	B
	ATOM	2492	NH1	ARG	B	446	72.878	-9.834	59.303	1.00	59.85	B
	ATOM	2493	NH2	ARG	B	446	73.677	-11.839	58.548	1.00	57.51	B
	ATOM	2494	C	ARG	B	446	74.712	-3.759	57.058	1.00	50.94	B
	ATOM	2495	O	ARG	B	446	73.764	-3.066	57.427	1.00	51.11	B
15	ATOM	2496	N	VAL	B	447	75.525	-3.414	56.063	1.00	49.98	B
	ATOM	2497	CA	VAL	B	447	75.338	-2.198	55.280	1.00	49.12	B
	ATOM	2498	CB	VAL	B	447	76.661	-1.360	55.196	1.00	49.77	B
	ATOM	2499	CG1	VAL	B	447	77.858	-2.268	55.110	1.00	48.80	B
	ATOM	2500	CG2	VAL	B	447	76.631	-0.433	53.984	1.00	50.29	B
20	ATOM	2501	C	VAL	B	447	74.876	-2.650	53.893	1.00	47.59	B
	ATOM	2502	O	VAL	B	447	75.433	-3.584	53.334	1.00	46.28	B
	ATOM	2503	N	TRP	B	448	73.841	-2.001	53.361	1.00	47.07	B
	ATOM	2504	CA	TRP	B	448	73.278	-2.349	52.058	1.00	46.70	B
	ATOM	2505	CB	TRP	B	448	71.807	-2.704	52.201	1.00	43.15	B
25	ATOM	2506	CG	TRP	B	448	71.506	-3.423	53.437	1.00	40.87	B
	ATOM	2507	CD2	TRP	B	448	71.126	-4.793	53.554	1.00	39.93	B
	ATOM	2508	CE2	TRP	B	448	70.984	-5.067	54.925	1.00	39.42	B
	ATOM	2509	CE3	TRP	B	448	70.907	-5.820	52.635	1.00	38.21	B
	ATOM	2510	CD1	TRP	B	448	71.565	-2.930	54.698	1.00	40.70	B
30	ATOM	2511	NE1	TRP	B	448	71.253	-3.910	55.603	1.00	40.18	B
	ATOM	2512	CZ2	TRP	B	448	70.620	-6.324	55.400	1.00	39.77	B
	ATOM	2513	CZ3	TRP	B	448	70.547	-7.073	53.110	1.00	38.97	B
	ATOM	2514	CH2	TRP	B	448	70.413	-7.314	54.480	1.00	38.38	B
	ATOM	2515	C	TRP	B	448	73.383	-1.223	51.038	1.00	48.93	B
35	ATOM	2516	O	TRP	B	448	73.774	-0.096	51.360	1.00	49.67	B
	ATOM	2517	N	ASP	B	449	73.001	-1.542	49.803	1.00	51.05	B
	ATOM	2518	CA	ASP	B	449	73.014	-0.586	48.698	1.00	52.47	B
	ATOM	2519	CB	ASP	B	449	74.247	-0.830	47.826	1.00	53.58	B
	ATOM	2520	CG	ASP	B	449	74.259	0.024	46.568	1.00	55.71	B
40	ATOM	2521	OD1	ASP	B	449	73.432	-0.234	45.662	1.00	56.14	B
	ATOM	2522	OD2	ASP	B	449	75.095	0.954	46.489	1.00	55.67	B
	ATOM	2523	C	ASP	B	449	71.733	-0.750	47.867	1.00	52.24	B
	ATOM	2524	O	ASP	B	449	71.541	-1.777	47.225	1.00	52.13	B
	ATOM	2525	N	ILE	B	450	70.864	0.260	47.883	1.00	52.28	B
45	ATOM	2526	CA	ILE	B	450	69.607	0.199	47.135	1.00	52.23	B
	ATOM	2527	CB	ILE	B	450	68.729	1.477	47.359	1.00	51.25	B
	ATOM	2528	CG2	ILE	B	450	67.411	1.352	46.609	1.00	50.40	B
	ATOM	2529	CG1	ILE	B	450	68.430	1.658	48.851	1.00	50.03	B
	ATOM	2530	CD1	ILE	B	450	67.617	2.890	49.180	1.00	49.00	B
50	ATOM	2531	C	ILE	B	450	69.849	0.024	45.639	1.00	52.47	B
	ATOM	2532	O	ILE	B	450	69.266	-0.860	45.024	1.00	52.87	B
	ATOM	2533	N	LYS	B	451	70.705	0.863	45.060	1.00	53.03	B
	ATOM	2534	CA	LYS	B	451	71.008	0.779	43.638	1.00	53.15	B
	ATOM	2535	CB	LYS	B	451	72.346	1.458	43.339	1.00	53.71	B

	ATOM	2536	CG	LYS	B	451	72.315	2.978	43.471	0.00	54.77	B
	ATOM	2537	CD	LYS	B	451	71.228	3.578	42.581	0.00	55.27	B
	ATOM	2538	CE	LYS	B	451	71.190	5.104	42.643	0.00	55.45	B
	ATOM	2539	NZ	LYS	B	451	72.286	5.761	41.877	0.00	55.61	B
5	ATOM	2540	C	LYS	B	451	71.059	-0.684	43.212	1.00	53.22	B
	ATOM	2541	O	LYS	B	451	70.241	-1.139	42.415	1.00	51.85	B
	ATOM	2542	N	LYS	B	452	72.007	-1.428	43.765	1.00	54.30	B
	ATOM	2543	CA	LYS	B	452	72.138	-2.833	43.431	1.00	55.55	B
	ATOM	2544	CB	LYS	B	452	73.549	-3.321	43.756	1.00	56.49	B
10	ATOM	2545	CG	LYS	B	452	74.596	-2.840	42.773	0.00	57.18	B
	ATOM	2546	CD	LYS	B	452	74.345	-3.420	41.393	0.00	57.78	B
	ATOM	2547	CE	LYS	B	452	75.353	-2.896	40.391	0.00	58.13	B
	ATOM	2548	NZ	LYS	B	452	75.066	-3.409	39.027	0.00	58.45	B
	ATOM	2549	C	LYS	B	452	71.113	-3.701	44.147	1.00	56.44	B
15	ATOM	2550	O	LYS	B	452	70.797	-4.790	43.679	1.00	58.17	B
	ATOM	2551	N	GLY	B	453	70.594	-3.234	45.279	1.00	56.96	B
	ATOM	2552	CA	GLY	B	453	69.605	-4.013	46.013	1.00	57.08	B
	ATOM	2553	C	GLY	B	453	70.167	-5.275	46.650	1.00	57.02	B
	ATOM	2554	O	GLY	B	453	69.573	-6.353	46.568	1.00	56.26	B
20	ATOM	2555	N	CYS	B	454	71.319	-5.143	47.297	1.00	57.42	B
	ATOM	2556	CA	CYS	B	454	71.958	-6.281	47.945	1.00	57.82	B
	ATOM	2557	CB	CYS	B	454	72.844	-7.024	46.937	1.00	59.05	B
	ATOM	2558	SG	CYS	B	454	74.118	-5.986	46.135	1.00	59.80	B
	ATOM	2559	C	CYS	B	454	72.800	-5.834	49.136	1.00	57.12	B
25	ATOM	2560	O	CYS	B	454	73.084	-4.644	49.300	1.00	57.22	B
	ATOM	2561	N	CYS	B	455	73.196	-6.798	49.961	1.00	55.66	B
	ATOM	2562	CA	CYS	B	455	74.021	-6.529	51.136	1.00	54.95	B
	ATOM	2563	CB	CYS	B	455	73.831	-7.667	52.140	1.00	54.92	B
	ATOM	2564	SG	CYS	B	455	74.504	-7.375	53.769	1.00	58.03	B
30	ATOM	2565	C	CYS	B	455	75.485	-6.436	50.678	1.00	54.21	B
	ATOM	2566	O	CYS	B	455	76.024	-7.404	50.146	1.00	55.39	B
	ATOM	2567	N	THR	B	456	76.120	-5.277	50.875	1.00	52.48	B
	ATOM	2568	CA	THR	B	456	77.514	-5.074	50.446	1.00	50.81	B
	ATOM	2569	CB	THR	B	456	77.771	-3.609	49.987	1.00	50.32	B
35	ATOM	2570	OG1	THR	B	456	77.631	-2.712	51.095	1.00	50.40	B
	ATOM	2571	CG2	THR	B	456	76.808	-3.217	48.894	1.00	49.71	B
	ATOM	2572	C	THR	B	456	78.608	-5.434	51.472	1.00	49.16	B
	ATOM	2573	O	THR	B	456	79.773	-5.613	51.109	1.00	49.26	B
	ATOM	2574	N	HIS	B	457	78.242	-5.537	52.743	1.00	46.55	B
40	ATOM	2575	CA	HIS	B	457	79.205	-5.871	53.780	1.00	43.83	B
	ATOM	2576	CB	HIS	B	457	79.956	-4.615	54.229	1.00	43.71	B
	ATOM	2577	CG	HIS	B	457	80.731	-3.947	53.136	1.00	44.34	B
	ATOM	2578	CD2	HIS	B	457	80.557	-2.753	52.524	1.00	44.60	B
	ATOM	2579	ND1	HIS	B	457	81.832	-4.524	52.543	1.00	44.61	B
45	ATOM	2580	CE1	HIS	B	457	82.305	-3.711	51.615	1.00	44.83	B
	ATOM	2581	NE2	HIS	B	457	81.550	-2.630	51.584	1.00	43.67	B
	ATOM	2582	C	HIS	B	457	78.512	-6.512	54.979	1.00	42.72	B
	ATOM	2583	O	HIS	B	457	77.307	-6.342	55.178	1.00	41.66	B
	ATOM	2584	N	VAL	B	458	79.275	-7.255	55.776	1.00	42.43	B
50	ATOM	2585	CA	VAL	B	458	78.725	-7.918	56.958	1.00	40.96	B
	ATOM	2586	CB	VAL	B	458	78.386	-9.383	56.655	1.00	41.12	B
	ATOM	2587	CG1	VAL	B	458	77.331	-9.883	57.628	1.00	39.96	B
	ATOM	2588	CG2	VAL	B	458	77.913	-9.519	55.225	1.00	40.46	B
	ATOM	2589	C	VAL	B	458	79.711	-7.852	58.130	1.00	39.97	B

	ATOM	2590	O	VAL	B	458	80.391	-8.820	58.456	1.00	38.56	B
	ATOM	2591	N	PHE	B	459	79.744	-6.690	58.768	1.00	40.60	B
	ATOM	2592	CA	PHE	B	459	80.623	-6.413	59.892	1.00	41.18	B
	ATOM	2593	CB	PHE	B	459	80.675	-4.901	60.084	1.00	38.09	B
5	ATOM	2594	CG	PHE	B	459	81.196	-4.158	58.881	1.00	36.10	B
	ATOM	2595	CD1	PHE	B	459	81.182	-2.765	58.850	1.00	34.95	B
	ATOM	2596	CD2	PHE	B	459	81.767	-4.847	57.813	1.00	34.29	B
	ATOM	2597	CE1	PHE	B	459	81.741	-2.055	57.773	1.00	34.55	B
	ATOM	2598	CE2	PHE	B	459	82.328	-4.160	56.734	1.00	35.73	B
10	ATOM	2599	CZ	PHE	B	459	82.317	-2.755	56.713	1.00	36.03	B
	ATOM	2600	C	PHE	B	459	80.237	-7.104	61.209	1.00	43.45	B
	ATOM	2601	O	PHE	B	459	79.357	-6.630	61.921	1.00	44.50	B
	ATOM	2602	N	GLU	B	460	80.900	-8.216	61.538	1.00	46.24	B
	ATOM	2603	CA	GLU	B	460	80.608	-8.939	62.783	1.00	47.21	B
15	ATOM	2604	CB	GLU	B	460	80.750	-10.456	62.599	1.00	46.96	B
	ATOM	2605	CG	GLU	B	460	79.920	-11.030	61.473	1.00	51.03	B
	ATOM	2606	CD	GLU	B	460	79.971	-12.553	61.386	1.00	52.17	B
	ATOM	2607	OE1	GLU	B	460	81.079	-13.110	61.261	1.00	54.35	B
	ATOM	2608	OE2	GLU	B	460	78.897	-13.194	61.428	1.00	51.82	B
20	ATOM	2609	C	GLU	B	460	81.532	-8.491	63.909	1.00	47.31	B
	ATOM	2610	O	GLU	B	460	82.567	-7.863	63.674	1.00	45.71	B
	ATOM	2611	N	GLY	B	461	81.147	-8.835	65.134	1.00	48.17	B
	ATOM	2612	CA	GLY	B	461	81.928	-8.456	66.292	1.00	49.82	B
	ATOM	2613	C	GLY	B	461	81.102	-8.363	67.561	1.00	50.83	B
25	ATOM	2614	O	GLY	B	461	81.379	-9.074	68.529	1.00	50.20	B
	ATOM	2615	N	HIS	B	462	80.086	-7.501	67.565	1.00	51.06	B
	ATOM	2616	CA	HIS	B	462	79.251	-7.346	68.750	1.00	51.73	B
	ATOM	2617	CB	HIS	B	462	78.010	-6.487	68.443	1.00	50.07	B
	ATOM	2618	CG	HIS	B	462	78.284	-5.011	68.421	1.00	48.90	B
30	ATOM	2619	CD2	HIS	B	462	78.451	-4.151	67.388	1.00	48.64	B
	ATOM	2620	ND1	HIS	B	462	78.443	-4.264	69.568	1.00	49.43	B
	ATOM	2621	CE1	HIS	B	462	78.697	-3.009	69.242	1.00	50.51	B
	ATOM	2622	NE2	HIS	B	462	78.708	-2.914	67.925	1.00	48.70	B
	ATOM	2623	C	HIS	B	462	78.846	-8.707	69.315	1.00	52.82	B
35	ATOM	2624	O	HIS	B	462	78.076	-9.459	68.704	1.00	53.62	B
	ATOM	2625	N	ASN	B	463	79.394	-9.013	70.490	1.00	53.69	B
	ATOM	2626	CA	ASN	B	463	79.140	-10.269	71.186	1.00	53.67	B
	ATOM	2627	CB	ASN	B	463	80.119	-10.413	72.369	0.00	53.95	B
	ATOM	2628	CG	ASN	B	463	81.588	-10.299	71.945	1.00	54.43	B
40	ATOM	2629	OD1	ASN	B	463	82.173	-11.235	71.378	1.00	55.63	B
	ATOM	2630	ND2	ASN	B	463	82.184	-9.140	72.216	1.00	52.98	B
	ATOM	2631	C	ASN	B	463	77.699	-10.312	71.686	1.00	53.05	B
	ATOM	2632	O	ASN	B	463	77.353	-11.133	72.525	1.00	53.74	B
	ATOM	2633	N	SER	B	464	76.867	-9.414	71.162	1.00	53.52	B
45	ATOM	2634	CA	SER	B	464	75.455	-9.330	71.540	1.00	51.56	B
	ATOM	2635	CB	SER	B	464	75.324	-8.732	72.946	1.00	52.15	B
	ATOM	2636	OG	SER	B	464	74.010	-8.925	73.444	1.00	54.03	B
	ATOM	2637	C	SER	B	464	74.645	-8.487	70.527	1.00	49.85	B
	ATOM	2638	O	SER	B	464	75.210	-7.852	69.622	1.00	47.81	B
50	ATOM	2639	N	THR	B	465	73.321	-8.496	70.695	1.00	48.25	B
	ATOM	2640	CA	THR	B	465	72.390	-7.767	69.824	1.00	47.13	B
	ATOM	2641	CB	THR	B	465	70.924	-7.847	70.344	1.00	48.31	B
	ATOM	2642	OG1	THR	B	465	70.510	-9.214	70.418	1.00	51.43	B
	ATOM	2643	CG2	THR	B	465	69.971	-7.098	69.412	1.00	49.57	B

	ATOM	2644	C	THR	B	465	72.734	-6.292	69.669	1.00	45.19	B
	ATOM	2645	O	THR	B	465	73.067	-5.617	70.643	1.00	45.46	B
	ATOM	2646	N	VAL	B	466	72.636	-5.804	68.433	1.00	42.21	B
	ATOM	2647	CA	VAL	B	466	72.912	-4.406	68.125	1.00	39.22	B
5	ATOM	2648	CB	VAL	B	466	73.293	-4.241	66.643	1.00	38.21	B
	ATOM	2649	CG1	VAL	B	466	73.798	-2.829	66.378	1.00	37.18	B
	ATOM	2650	CG2	VAL	B	466	74.354	-5.264	66.285	1.00	35.99	B
	ATOM	2651	C	VAL	B	466	71.626	-3.638	68.430	1.00	37.88	B
	ATOM	2652	O	VAL	B	466	70.655	-3.738	67.691	1.00	35.76	B
10	ATOM	2653	N	ARG	B	467	71.623	-2.886	69.530	1.00	37.28	B
	ATOM	2654	CA	ARG	B	467	70.440	-2.145	69.938	1.00	36.20	B
	ATOM	2655	CB	ARG	B	467	70.399	-1.987	71.468	1.00	36.76	B
	ATOM	2656	CG	ARG	B	467	69.038	-1.513	72.012	1.00	36.98	B
	ATOM	2657	CD	ARG	B	467	67.945	-2.559	71.762	1.00	39.61	B
15	ATOM	2658	NE	ARG	B	467	66.563	-2.103	71.979	1.00	40.08	B
	ATOM	2659	CZ	ARG	B	467	65.928	-1.213	71.220	1.00	38.58	B
	ATOM	2660	NH1	ARG	B	467	66.539	-0.654	70.184	1.00	36.43	B
	ATOM	2661	NH2	ARG	B	467	64.664	-0.913	71.476	1.00	39.24	B
	ATOM	2662	C	ARG	B	467	70.314	-0.773	69.283	1.00	35.21	B
20	ATOM	2663	O	ARG	B	467	69.225	-0.213	69.247	1.00	36.67	B
	ATOM	2664	N	CYS	B	468	71.400	-0.222	68.758	1.00	33.04	B
	ATOM	2665	CA	CYS	B	468	71.304	1.088	68.127	1.00	33.09	B
	ATOM	2666	CB	CYS	B	468	71.069	2.167	69.186	1.00	32.72	B
	ATOM	2667	SG	CYS	B	468	72.414	2.394	70.339	1.00	34.24	B
25	ATOM	2668	C	CYS	B	468	72.533	1.406	67.292	1.00	32.45	B
	ATOM	2669	O	CYS	B	468	73.473	0.618	67.263	1.00	33.24	B
	ATOM	2670	N	LEU	B	469	72.522	2.546	66.605	1.00	31.75	B
	ATOM	2671	CA	LEU	B	469	73.643	2.908	65.747	1.00	32.36	B
	ATOM	2672	CB	LEU	B	469	73.750	1.917	64.576	1.00	32.24	B
30	ATOM	2673	CG	LEU	B	469	72.822	2.067	63.362	1.00	31.67	B
	ATOM	2674	CD1	LEU	B	469	73.563	2.673	62.174	1.00	33.01	B
	ATOM	2675	CD2	LEU	B	469	72.311	0.704	62.982	1.00	33.19	B
	ATOM	2676	C	LEU	B	469	73.491	4.309	65.179	1.00	32.21	B
	ATOM	2677	O	LEU	B	469	72.434	4.910	65.285	1.00	32.62	B
35	ATOM	2678	N	ASP	B	470	74.552	4.833	64.581	1.00	33.12	B
	ATOM	2679	CA	ASP	B	470	74.481	6.149	63.972	1.00	34.33	B
	ATOM	2680	CB	ASP	B	470	74.431	7.223	65.055	1.00	33.47	B
	ATOM	2681	CG	ASP	B	470	74.098	8.585	64.501	1.00	32.01	B
	ATOM	2682	OD1	ASP	B	470	73.302	8.647	63.551	1.00	35.18	B
40	ATOM	2683	OD2	ASP	B	470	74.614	9.589	65.021	1.00	29.33	B
	ATOM	2684	C	ASP	B	470	75.704	6.330	63.083	1.00	35.86	B
	ATOM	2685	O	ASP	B	470	76.619	5.509	63.124	1.00	36.56	B
	ATOM	2686	N	ILE	B	471	75.712	7.384	62.269	1.00	37.44	B
	ATOM	2687	CA	ILE	B	471	76.841	7.663	61.380	1.00	37.88	B
45	ATOM	2688	CB	ILE	B	471	76.465	7.465	59.889	1.00	36.84	B
	ATOM	2689	CG2	ILE	B	471	77.698	7.683	59.005	1.00	36.56	B
	ATOM	2690	CG1	ILE	B	471	75.942	6.050	59.649	1.00	36.63	B
	ATOM	2691	CD1	ILE	B	471	75.305	5.868	58.283	1.00	35.99	B
	ATOM	2692	C	ILE	B	471	77.309	9.106	61.569	1.00	38.95	B
50	ATOM	2693	O	ILE	B	471	76.493	10.013	61.769	1.00	39.67	B
	ATOM	2694	N	VAL	B	472	78.625	9.305	61.522	1.00	39.62	B
	ATOM	2695	CA	VAL	B	472	79.219	10.631	61.670	1.00	40.41	B
	ATOM	2696	CB	VAL	B	472	79.932	10.786	63.018	1.00	39.84	B
	ATOM	2697	CG1	VAL	B	472	78.967	10.468	64.158	1.00	37.97	B

	ATOM	2698	CG2	VAL	B	472	81.150	9.862	63.066	1.00	38.84	B
	ATOM	2699	C	VAL	B	472	80.255	10.802	60.579	1.00	42.22	B
	ATOM	2700	O	VAL	B	472	80.780	9.820	60.064	1.00	41.41	B
	ATOM	2701	N	GLU	B	473	80.544	12.048	60.227	1.00	44.76	B
5	ATOM	2702	CA	GLU	B	473	81.539	12.329	59.207	1.00	48.54	B
	ATOM	2703	CB	GLU	B	473	80.872	12.865	57.934	1.00	49.21	B
	ATOM	2704	CG	GLU	B	473	81.851	13.193	56.784	1.00	51.32	B
	ATOM	2705	CD	GLU	B	473	81.143	13.514	55.465	1.00	51.78	B
	ATOM	2706	OE1	GLU	B	473	80.489	12.609	54.902	1.00	52.52	B
10	ATOM	2707	OE2	GLU	B	473	81.232	14.670	54.996	1.00	52.59	B
	ATOM	2708	C	GLU	B	473	82.568	13.329	59.737	1.00	50.91	B
	ATOM	2709	O	GLU	B	473	82.225	14.419	60.205	1.00	50.21	B
	ATOM	2710	N	TYR	B	474	83.835	12.933	59.683	1.00	53.85	B
	ATOM	2711	CA	TYR	B	474	84.927	13.775	60.151	1.00	56.31	B
15	ATOM	2712	CB	TYR	B	474	85.504	13.214	61.450	1.00	57.48	B
	ATOM	2713	CG	TYR	B	474	86.410	14.180	62.164	1.00	59.70	B
	ATOM	2714	CD1	TYR	B	474	85.925	15.408	62.613	1.00	60.47	B
	ATOM	2715	CE1	TYR	B	474	86.744	16.305	63.285	1.00	60.97	B
	ATOM	2716	CD2	TYR	B	474	87.749	13.870	62.402	1.00	60.68	B
20	ATOM	2717	CE2	TYR	B	474	88.581	14.763	63.075	1.00	61.50	B
	ATOM	2718	CZ	TYR	B	474	88.068	15.978	63.514	1.00	61.92	B
	ATOM	2719	OH	TYR	B	474	88.875	16.861	64.194	1.00	63.90	B
	ATOM	2720	C	TYR	B	474	86.001	13.795	59.075	1.00	56.54	B
	ATOM	2721	O	TYR	B	474	86.293	12.768	58.460	1.00	56.18	B
25	ATOM	2722	N	LYS	B	475	86.589	14.966	58.856	1.00	58.01	B
	ATOM	2723	CA	LYS	B	475	87.623	15.128	57.840	1.00	59.54	B
	ATOM	2724	CB	LYS	B	475	88.958	14.579	58.351	1.00	60.12	B
	ATOM	2725	CG	LYS	B	475	89.453	15.213	59.653	1.00	60.74	B
	ATOM	2726	CD	LYS	B	475	89.934	16.642	59.449	1.00	61.48	B
30	ATOM	2727	CE	LYS	B	475	90.341	17.283	60.765	0.00	61.92	B
	ATOM	2728	NZ	LYS	B	475	90.797	18.687	60.568	0.00	62.37	B
	ATOM	2729	C	LYS	B	475	87.200	14.393	56.563	1.00	60.31	B
	ATOM	2730	O	LYS	B	475	87.882	13.481	56.093	1.00	61.02	B
	ATOM	2731	N	ASN	B	476	86.057	14.796	56.020	1.00	60.89	B
35	ATOM	2732	CA	ASN	B	476	85.523	14.199	54.813	1.00	60.87	B
	ATOM	2733	CB	ASN	B	476	86.260	14.759	53.594	1.00	63.50	B
	ATOM	2734	CG	ASN	B	476	85.792	16.172	53.224	1.00	66.46	B
	ATOM	2735	OD1	ASN	B	476	84.649	16.361	52.785	1.00	68.68	B
	ATOM	2736	ND2	ASN	B	476	86.668	17.167	53.405	1.00	65.78	B
40	ATOM	2737	C	ASN	B	476	85.593	12.676	54.843	1.00	60.30	B
	ATOM	2738	O	ASN	B	476	85.828	12.036	53.822	1.00	61.52	B
	ATOM	2739	N	ILE	B	477	85.379	12.095	56.018	1.00	58.81	B
	ATOM	2740	CA	ILE	B	477	85.395	10.642	56.155	1.00	57.40	B
	ATOM	2741	CB	ILE	B	477	86.720	10.148	56.780	1.00	58.27	B
45	ATOM	2742	CG2	ILE	B	477	86.741	8.618	56.804	1.00	58.03	B
	ATOM	2743	CG1	ILE	B	477	87.903	10.659	55.960	0.00	58.14	B
	ATOM	2744	CD1	ILE	B	477	89.253	10.422	56.599	0.00	58.25	B
	ATOM	2745	C	ILE	B	477	84.224	10.183	57.030	1.00	55.59	B
	ATOM	2746	O	ILE	B	477	84.050	10.661	58.151	1.00	55.65	B
50	ATOM	2747	N	LYS	B	478	83.423	9.257	56.515	1.00	52.92	B
	ATOM	2748	CA	LYS	B	478	82.281	8.760	57.264	1.00	51.69	B
	ATOM	2749	CB	LYS	B	478	81.106	8.479	56.322	1.00	50.04	B
	ATOM	2750	CG	LYS	B	478	80.324	9.717	55.899	1.00	47.12	B
	ATOM	2751	CD	LYS	B	478	78.972	9.329	55.324	1.00	46.70	B

	ATOM	2752	CE	LYS	B	478	78.106	10.553	55.048	1.00	45.79	B
	ATOM	2753	NZ	LYS	B	478	76.681	10.181	54.803	1.00	44.56	B
	ATOM	2754	C	LYS	B	478	82.591	7.509	58.090	1.00	52.07	B
	ATOM	2755	O	LYS	B	478	83.279	6.593	57.620	1.00	53.19	B
5	ATOM	2756	N	TYR	B	479	82.076	7.485	59.323	1.00	51.09	B
	ATOM	2757	CA	TYR	B	479	82.273	6.363	60.250	1.00	49.59	B
	ATOM	2758	CB	TYR	B	479	83.083	6.815	61.492	1.00	50.00	B
	ATOM	2759	CG	TYR	B	479	84.438	7.442	61.183	1.00	49.78	B
	ATOM	2760	CD1	TYR	B	479	84.526	8.594	60.402	1.00	50.71	B
10	ATOM	2761	CE1	TYR	B	479	85.754	9.165	60.062	1.00	49.52	B
	ATOM	2762	CD2	TYR	B	479	85.629	6.869	61.630	1.00	49.70	B
	ATOM	2763	CE2	TYR	B	479	86.870	7.438	61.291	1.00	49.93	B
	ATOM	2764	CZ	TYR	B	479	86.918	8.586	60.502	1.00	49.57	B
	ATOM	2765	OH	TYR	B	479	88.115	9.155	60.126	1.00	48.42	B
15	ATOM	2766	C	TYR	B	479	80.922	5.790	60.698	1.00	48.39	B
	ATOM	2767	O	TYR	B	479	79.877	6.381	60.463	1.00	47.95	B
	ATOM	2768	N	ILE	B	480	80.954	4.629	61.337	1.00	48.14	B
	ATOM	2769	CA	ILE	B	480	79.742	3.986	61.828	1.00	47.98	B
	ATOM	2770	CB	ILE	B	480	79.470	2.669	61.090	1.00	47.82	B
20	ATOM	2771	CG2	ILE	B	480	78.250	1.983	61.679	1.00	48.23	B
	ATOM	2772	CG1	ILE	B	480	79.275	2.929	59.599	1.00	47.92	B
	ATOM	2773	CD1	ILE	B	480	79.279	1.675	58.768	1.00	46.66	B
	ATOM	2774	C	ILE	B	480	79.930	3.651	63.308	1.00	48.77	B
	ATOM	2775	O	ILE	B	480	80.961	3.089	63.699	1.00	49.54	B
25	ATOM	2776	N	VAL	B	481	78.931	3.982	64.124	1.00	48.38	B
	ATOM	2777	CA	VAL	B	481	78.975	3.718	65.566	1.00	46.50	B
	ATOM	2778	CB	VAL	B	481	78.917	5.041	66.382	1.00	46.27	B
	ATOM	2779	CG1	VAL	B	481	79.048	4.749	67.871	1.00	44.39	B
	ATOM	2780	CG2	VAL	B	481	80.004	5.990	65.914	1.00	45.50	B
30	ATOM	2781	C	VAL	B	481	77.778	2.855	65.962	1.00	45.57	B
	ATOM	2782	O	VAL	B	481	76.634	3.281	65.823	1.00	45.94	B
	ATOM	2783	N	THR	B	482	78.039	1.652	66.460	1.00	43.78	B
	ATOM	2784	CA	THR	B	482	76.963	0.752	66.865	1.00	43.35	B
	ATOM	2785	CB	THR	B	482	77.050	-0.608	66.091	1.00	44.57	B
35	ATOM	2786	OG1	THR	B	482	78.422	-0.943	65.851	1.00	44.68	B
	ATOM	2787	CG2	THR	B	482	76.315	-0.523	64.748	1.00	44.18	B
	ATOM	2788	C	THR	B	482	76.946	0.475	68.379	1.00	42.32	B
	ATOM	2789	O	THR	B	482	77.979	0.184	68.977	1.00	42.34	B
	ATOM	2790	N	GLY	B	483	75.769	0.583	68.991	1.00	41.18	B
40	ATOM	2791	CA	GLY	B	483	75.643	0.319	70.410	1.00	42.21	B
	ATOM	2792	C	GLY	B	483	75.021	-1.057	70.556	1.00	43.25	B
	ATOM	2793	O	GLY	B	483	74.069	-1.385	69.837	1.00	44.15	B
	ATOM	2794	N	SER	B	484	75.536	-1.865	71.479	1.00	42.55	B
	ATOM	2795	CA	SER	B	484	75.018	-3.216	71.650	1.00	42.61	B
45	ATOM	2796	CB	SER	B	484	76.015	-4.236	71.071	1.00	42.00	B
	ATOM	2797	OG	SER	B	484	75.676	-5.572	71.425	1.00	39.48	B
	ATOM	2798	C	SER	B	484	74.721	-3.560	73.099	1.00	43.04	B
	ATOM	2799	O	SER	B	484	75.118	-2.833	74.007	1.00	43.14	B
	ATOM	2800	N	ARG	B	485	73.993	-4.664	73.294	1.00	43.38	B
50	ATOM	2801	CA	ARG	B	485	73.628	-5.182	74.618	1.00	42.66	B
	ATOM	2802	CB	ARG	B	485	72.532	-6.233	74.484	1.00	41.35	B
	ATOM	2803	CG	ARG	B	485	71.309	-5.751	73.737	1.00	41.63	B
	ATOM	2804	CD	ARG	B	485	70.170	-5.535	74.696	1.00	40.30	B
	ATOM	2805	NE	ARG	B	485	69.101	-6.499	74.462	1.00	41.39	B

	ATOM	2806	CZ	ARG	B	485	67.859	-6.154	74.146	1.00	42.42	B
	ATOM	2807	NH1	ARG	B	485	67.547	-4.874	74.029	1.00	44.59	B
	ATOM	2808	NH2	ARG	B	485	66.927	-7.076	73.964	1.00	41.56	B
	ATOM	2809	C	ARG	B	485	74.879	-5.837	75.200	1.00	43.12	B
5	ATOM	2810	O	ARG	B	485	74.845	-6.448	76.264	1.00	42.36	B
	ATOM	2811	N	ASP	B	486	75.974	-5.714	74.463	1.00	43.89	B
	ATOM	2812	CA	ASP	B	486	77.232	-6.263	74.880	1.00	44.86	B
	ATOM	2813	CB	ASP	B	486	78.100	-6.572	73.646	1.00	45.64	B
	ATOM	2814	CG	ASP	B	486	78.713	-5.327	73.012	1.00	46.63	B
10	ATOM	2815	OD1	ASP	B	486	78.016	-4.298	72.888	1.00	46.93	B
	ATOM	2816	OD2	ASP	B	486	79.897	-5.387	72.619	1.00	47.67	B
	ATOM	2817	C	ASP	B	486	77.887	-5.242	75.807	1.00	45.67	B
	ATOM	2818	O	ASP	B	486	78.967	-5.486	76.344	1.00	46.05	B
	ATOM	2819	N	ASN	B	487	77.207	-4.108	76.003	1.00	45.49	B
15	ATOM	2820	CA	ASN	B	487	77.673	-3.017	76.873	1.00	44.88	B
	ATOM	2821	CB	ASN	B	487	78.223	-3.571	78.188	1.00	44.56	B
	ATOM	2822	CG	ASN	B	487	77.171	-4.261	79.021	1.00	45.76	B
	ATOM	2823	OD1	ASN	B	487	76.153	-4.717	78.508	1.00	47.63	B
	ATOM	2824	ND2	ASN	B	487	77.421	-4.359	80.317	1.00	45.91	B
20	ATOM	2825	C	ASN	B	487	78.748	-2.146	76.242	1.00	44.09	B
	ATOM	2826	O	ASN	B	487	79.333	-1.306	76.920	1.00	43.58	B
	ATOM	2827	N	THR	B	488	79.009	-2.347	74.953	1.00	44.03	B
	ATOM	2828	CA	THR	B	488	80.038	-1.576	74.267	1.00	45.88	B
	ATOM	2829	CB	THR	B	488	81.264	-2.458	73.895	1.00	46.72	B
25	ATOM	2830	OG1	THR	B	488	81.026	-3.098	72.633	1.00	46.03	B
	ATOM	2831	CG2	THR	B	488	81.498	-3.545	74.958	1.00	47.35	B
	ATOM	2832	C	THR	B	488	79.525	-0.958	72.971	1.00	46.36	B
	ATOM	2833	O	THR	B	488	78.403	-1.224	72.542	1.00	47.28	B
	ATOM	2834	N	LEU	B	489	80.369	-0.135	72.355	1.00	45.88	B
30	ATOM	2835	CA	LEU	B	489	80.053	0.511	71.090	1.00	46.03	B
	ATOM	2836	CB	LEU	B	489	79.848	2.015	71.269	1.00	45.02	B
	ATOM	2837	CG	LEU	B	489	78.651	2.443	72.110	1.00	44.47	B
	ATOM	2838	CD1	LEU	B	489	79.093	2.732	73.518	1.00	43.21	B
	ATOM	2839	CD2	LEU	B	489	78.011	3.655	71.484	1.00	45.05	B
35	ATOM	2840	C	LEU	B	489	81.186	0.293	70.102	1.00	47.37	B
	ATOM	2841	O	LEU	B	489	82.281	0.840	70.280	1.00	48.75	B
	ATOM	2842	N	HIS	B	490	80.930	-0.507	69.067	1.00	46.28	B
	ATOM	2843	CA	HIS	B	490	81.940	-0.766	68.040	1.00	44.43	B
	ATOM	2844	CB	HIS	B	490	81.680	-2.105	67.363	1.00	46.31	B
40	ATOM	2845	CG	HIS	B	490	81.979	-3.288	68.226	1.00	48.42	B
	ATOM	2846	CD2	HIS	B	490	82.601	-4.456	67.944	1.00	48.94	B
	ATOM	2847	ND1	HIS	B	490	81.584	-3.371	69.544	1.00	48.72	B
	ATOM	2848	CE1	HIS	B	490	81.947	-4.542	70.035	1.00	48.74	B
	ATOM	2849	NE2	HIS	B	490	82.566	-5.220	69.084	1.00	49.32	B
45	ATOM	2850	C	HIS	B	490	81.932	0.332	66.988	1.00	41.63	B
	ATOM	2851	O	HIS	B	490	80.873	0.804	66.598	1.00	39.88	B
	ATOM	2852	N	VAL	B	491	83.119	0.727	66.537	1.00	41.79	B
	ATOM	2853	CA	VAL	B	491	83.268	1.774	65.523	1.00	43.45	B
	ATOM	2854	CB	VAL	B	491	84.258	2.873	65.987	1.00	43.37	B
50	ATOM	2855	CG1	VAL	B	491	84.565	3.838	64.843	1.00	43.14	B
	ATOM	2856	CG2	VAL	B	491	83.661	3.642	67.158	1.00	42.84	B
	ATOM	2857	C	VAL	B	491	83.773	1.199	64.201	1.00	43.94	B
	ATOM	2858	O	VAL	B	491	84.794	0.515	64.165	1.00	45.06	B
	ATOM	2859	N	TRP	B	492	83.056	1.479	63.115	1.00	44.26	B

	ATOM	2860	CA	TRP	B	492	83.453	0.982	61.804	1.00	43.81	B
	ATOM	2861	CB	TRP	B	492	82.481	-0.086	61.312	1.00	42.52	B
	ATOM	2862	CG	TRP	B	492	81.869	-0.922	62.399	1.00	42.97	B
	ATOM	2863	CD2	TRP	B	492	82.119	-2.308	62.661	1.00	43.02	B
5	ATOM	2864	CE2	TRP	B	492	81.258	-2.696	63.721	1.00	42.64	B
	ATOM	2865	CE3	TRP	B	492	82.980	-3.262	62.102	1.00	42.84	B
	ATOM	2866	CD1	TRP	B	492	80.906	-0.535	63.289	1.00	42.27	B
	ATOM	2867	NE1	TRP	B	492	80.532	-1.593	64.081	1.00	42.22	B
	ATOM	2868	CZ2	TRP	B	492	81.231	-4.000	64.235	1.00	43.33	B
10	ATOM	2869	CZ3	TRP	B	492	82.955	-4.562	62.613	1.00	43.23	B
	ATOM	2870	CH2	TRP	B	492	82.083	-4.917	63.670	1.00	43.67	B
	ATOM	2871	C	TRP	B	492	83.493	2.123	60.804	1.00	44.22	B
	ATOM	2872	O	TRP	B	492	83.061	3.233	61.094	1.00	43.90	B
	ATOM	2873	N	LYS	B	493	84.033	1.847	59.627	1.00	45.31	B
15	ATOM	2874	CA	LYS	B	493	84.115	2.855	58.596	1.00	46.28	B
	ATOM	2875	CB	LYS	B	493	85.515	2.896	57.997	1.00	47.20	B
	ATOM	2876	CG	LYS	B	493	86.600	3.104	59.021	1.00	48.93	B
	ATOM	2877	CD	LYS	B	493	87.962	3.179	58.363	0.00	48.94	B
	ATOM	2878	CE	LYS	B	493	89.061	3.374	59.394	0.00	49.30	B
20	ATOM	2879	NZ	LYS	B	493	90.390	3.550	58.746	0.00	49.52	B
	ATOM	2880	C	LYS	B	493	83.108	2.522	57.518	1.00	47.32	B
	ATOM	2881	O	LYS	B	493	82.863	1.349	57.220	1.00	47.63	B
	ATOM	2882	N	LEU	B	494	82.514	3.563	56.952	1.00	47.99	B
	ATOM	2883	CA	LEU	B	494	81.539	3.395	55.895	1.00	48.33	B
25	ATOM	2884	CB	LEU	B	494	80.733	4.674	55.717	1.00	48.56	B
	ATOM	2885	CG	LEU	B	494	79.698	4.594	54.604	1.00	48.11	B
	ATOM	2886	CD1	LEU	B	494	78.587	3.650	55.032	1.00	47.88	B
	ATOM	2887	CD2	LEU	B	494	79.156	5.988	54.313	1.00	49.20	B
	ATOM	2888	C	LEU	B	494	82.298	3.086	54.618	1.00	48.60	B
30	ATOM	2889	O	LEU	B	494	83.009	3.938	54.096	1.00	48.84	B
	ATOM	2890	N	PRO	B	495	82.170	1.856	54.109	1.00	48.59	B
	ATOM	2891	CD	PRO	B	495	81.485	0.713	54.729	1.00	48.94	B
	ATOM	2892	CA	PRO	B	495	82.850	1.438	52.887	1.00	50.38	B
	ATOM	2893	CB	PRO	B	495	82.345	0.014	52.693	1.00	49.35	B
35	ATOM	2894	CG	PRO	B	495	82.201	-0.461	54.107	1.00	48.48	B
	ATOM	2895	C	PRO	B	495	82.561	2.342	51.693	1.00	52.37	B
	ATOM	2896	O	PRO	B	495	81.415	2.741	51.456	1.00	53.23	B
	ATOM	2897	N	LYS	B	496	83.625	2.669	50.963	1.00	53.80	B
	ATOM	2898	CA	LYS	B	496	83.557	3.519	49.784	1.00	54.63	B
40	ATOM	2899	CB	LYS	B	496	84.934	4.155	49.529	1.00	55.28	B
	ATOM	2900	CG	LYS	B	496	86.118	3.196	49.670	1.00	54.90	B
	ATOM	2901	CD	LYS	B	496	87.443	3.945	49.624	1.00	54.86	B
	ATOM	2902	CE	LYS	B	496	88.625	3.017	49.840	0.00	55.42	B
	ATOM	2903	NZ	LYS	B	496	89.917	3.759	49.828	0.00	55.70	B
45	ATOM	2904	C	LYS	B	496	83.100	2.731	48.559	1.00	54.70	B
	ATOM	2905	O	LYS	B	496	82.693	3.317	47.553	1.00	54.41	B
	ATOM	2906	N	ASP	B	508	80.076	-10.950	44.143	1.00	87.67	B
	ATOM	2907	CA	ASP	B	508	81.314	-10.630	44.843	1.00	87.56	B
	ATOM	2908	CB	ASP	B	508	82.398	-10.224	43.855	1.00	85.57	B
50	ATOM	2909	CG	ASP	B	508	82.370	-8.742	43.565	1.00	84.40	B
	ATOM	2910	OD1	ASP	B	508	81.334	-8.260	43.072	1.00	83.24	B
	ATOM	2911	OD2	ASP	B	508	83.371	-8.056	43.855	1.00	83.59	B
	ATOM	2912	C	ASP	B	508	81.080	-9.451	45.781	1.00	88.88	B
	ATOM	2913	O	ASP	B	508	82.036	-8.810	46.225	1.00	89.19	B

	ATOM	2914	N	TYR	B	509	79.812	-9.155	46.066	1.00	89.80	B
	ATOM	2915	CA	TYR	B	509	79.455	-8.033	46.939	1.00	89.61	B
	ATOM	2916	CB	TYR	B	509	78.210	-7.309	46.397	1.00	90.86	B
	ATOM	2917	CG	TYR	B	509	78.488	-5.981	45.705	1.00	92.99	B
5	ATOM	2918	CD1	TYR	B	509	77.576	-5.455	44.774	1.00	94.09	B
	ATOM	2919	CE1	TYR	B	509	77.817	-4.236	44.120	1.00	94.93	B
	ATOM	2920	CD2	TYR	B	509	79.653	-5.252	45.974	1.00	93.03	B
	ATOM	2921	CE2	TYR	B	509	79.906	-4.032	45.329	1.00	94.38	B
	ATOM	2922	CZ	TYR	B	509	78.986	-3.530	44.401	1.00	95.32	B
10	ATOM	2923	OH	TYR	B	509	79.241	-2.342	43.743	1.00	95.61	B
	ATOM	2924	C	TYR	B	509	79.236	-8.425	48.404	1.00	88.37	B
	ATOM	2925	O	TYR	B	509	79.772	-7.770	49.301	1.00	89.80	B
	ATOM	2926	N	PRO	B	510	78.448	-9.487	48.672	1.00	86.15	B
	ATOM	2927	CD	PRO	B	510	77.598	-10.261	47.751	1.00	84.82	B
15	ATOM	2928	CA	PRO	B	510	78.214	-9.897	50.067	1.00	83.98	B
	ATOM	2929	CB	PRO	B	510	77.276	-11.093	49.923	1.00	84.08	B
	ATOM	2930	CG	PRO	B	510	76.518	-10.763	48.676	1.00	84.98	B
	ATOM	2931	C	PRO	B	510	79.508	-10.265	50.800	1.00	81.81	B
	ATOM	2932	O	PRO	B	510	79.788	-11.441	51.017	1.00	81.76	B
20	ATOM	2933	N	LEU	B	511	80.289	-9.254	51.176	1.00	79.52	B
	ATOM	2934	CA	LEU	B	511	81.556	-9.462	51.875	1.00	77.45	B
	ATOM	2935	CB	LEU	B	511	82.466	-8.246	51.701	1.00	75.86	B
	ATOM	2936	CG	LEU	B	511	82.803	-7.866	50.264	1.00	74.15	B
	ATOM	2937	CD1	LEU	B	511	83.709	-6.653	50.229	1.00	72.84	B
25	ATOM	2938	CD2	LEU	B	511	83.463	-9.053	49.601	1.00	74.63	B
	ATOM	2939	C	LEU	B	511	81.323	-9.689	53.355	1.00	77.25	B
	ATOM	2940	O	LEU	B	511	80.682	-8.878	54.020	1.00	77.95	B
	ATOM	2941	N	VAL	B	512	81.856	-10.785	53.877	1.00	76.40	B
	ATOM	2942	CA	VAL	B	512	81.683	-11.100	55.286	1.00	75.66	B
30	ATOM	2943	CB	VAL	B	512	81.075	-12.495	55.458	1.00	74.68	B
	ATOM	2944	CG1	VAL	B	512	80.748	-12.736	56.917	1.00	73.65	B
	ATOM	2945	CG2	VAL	B	512	79.843	-12.625	54.587	1.00	73.90	B
	ATOM	2946	C	VAL	B	512	83.009	-11.040	56.029	1.00	75.90	B
	ATOM	2947	O	VAL	B	512	84.015	-11.558	55.560	1.00	76.65	B
35	ATOM	2948	N	PHE	B	513	83.007	-10.394	57.187	1.00	75.87	B
	ATOM	2949	CA	PHE	B	513	84.218	-10.275	57.986	1.00	75.67	B
	ATOM	2950	CB	PHE	B	513	84.669	-8.820	58.058	1.00	74.40	B
	ATOM	2951	CG	PHE	B	513	84.758	-8.148	56.722	1.00	74.06	B
	ATOM	2952	CD1	PHE	B	513	83.611	-7.885	55.981	1.00	74.40	B
40	ATOM	2953	CD2	PHE	B	513	85.987	-7.765	56.208	1.00	74.00	B
	ATOM	2954	CE1	PHE	B	513	83.686	-7.246	54.752	1.00	74.32	B
	ATOM	2955	CE2	PHE	B	513	86.077	-7.126	54.979	1.00	73.93	B
	ATOM	2956	CZ	PHE	B	513	84.921	-6.865	54.249	1.00	74.51	B
	ATOM	2957	C	PHE	B	513	83.893	-10.780	59.378	1.00	76.17	B
45	ATOM	2958	O	PHE	B	513	83.367	-10.041	60.207	1.00	76.66	B
	ATOM	2959	N	HIS	B	514	84.203	-12.043	59.631	1.00	76.08	B
	ATOM	2960	CA	HIS	B	514	83.906	-12.636	60.919	1.00	76.38	B
	ATOM	2961	CB	HIS	B	514	83.697	-14.139	60.758	1.00	78.44	B
	ATOM	2962	CG	HIS	B	514	84.803	-14.820	60.022	1.00	81.60	B
50	ATOM	2963	CD2	HIS	B	514	85.579	-15.876	60.360	1.00	82.68	B
	ATOM	2964	ND1	HIS	B	514	85.232	-14.407	58.780	1.00	82.91	B
	ATOM	2965	CE1	HIS	B	514	86.228	-15.180	58.384	1.00	84.06	B
	ATOM	2966	NE2	HIS	B	514	86.458	-16.079	59.324	1.00	83.92	B
	ATOM	2967	C	HIS	B	514	84.981	-12.355	61.948	1.00	75.65	B

	ATOM	2968	O	HIS	B	514	84.997	-12.964	63.016	1.00	75.17	B
	ATOM	2969	N	THR	B	515	85.880	-11.431	61.632	1.00	75.12	B
	ATOM	2970	CA	THR	B	515	86.931	-11.076	62.573	1.00	75.68	B
	ATOM	2971	CB	THR	B	515	88.219	-11.871	62.315	1.00	75.87	B
5	ATOM	2972	OG1	THR	B	515	87.936	-13.276	62.363	1.00	75.87	B
	ATOM	2973	CG2	THR	B	515	89.255	-11.538	63.375	1.00	74.95	B
	ATOM	2974	C	THR	B	515	87.245	-9.590	62.492	1.00	75.55	B
	ATOM	2975	O	THR	B	515	87.642	-9.087	61.445	1.00	75.60	B
	ATOM	2976	N	PRO	B	516	87.061	-8.869	63.606	1.00	75.61	B
10	ATOM	2977	CD	PRO	B	516	86.520	-9.405	64.867	1.00	76.30	B
	ATOM	2978	CA	PRO	B	516	87.308	-7.430	63.722	1.00	75.87	B
	ATOM	2979	CB	PRO	B	516	87.056	-7.161	65.202	1.00	76.07	B
	ATOM	2980	CG	PRO	B	516	86.008	-8.162	65.550	1.00	76.54	B
	ATOM	2981	C	PRO	B	516	88.719	-7.025	63.299	1.00	76.37	B
15	ATOM	2982	O	PRO	B	516	88.897	-6.183	62.415	1.00	75.84	B
	ATOM	2983	N	GLU	B	517	89.714	-7.626	63.949	1.00	76.93	B
	ATOM	2984	CA	GLU	B	517	91.126	-7.356	63.676	1.00	76.76	B
	ATOM	2985	CB	GLU	B	517	91.996	-8.320	64.492	1.00	78.63	B
	ATOM	2986	CG	GLU	B	517	93.496	-8.083	64.384	1.00	81.28	B
20	ATOM	2987	CD	GLU	B	517	93.944	-6.839	65.123	1.00	82.27	B
	ATOM	2988	OE1	GLU	B	517	95.171	-6.593	65.192	1.00	83.01	B
	ATOM	2989	OE2	GLU	B	517	93.066	-6.107	65.630	1.00	82.62	B
	ATOM	2990	C	GLU	B	517	91.448	-7.505	62.189	1.00	75.46	B
	ATOM	2991	O	GLU	B	517	92.318	-6.812	61.663	1.00	75.08	B
25	ATOM	2992	N	GLU	B	518	90.733	-8.411	61.525	1.00	73.54	B
	ATOM	2993	CA	GLU	B	518	90.927	-8.681	60.106	1.00	71.48	B
	ATOM	2994	CB	GLU	B	518	90.530	-10.124	59.793	0.00	72.44	B
	ATOM	2995	CG	GLU	B	518	90.797	-10.526	58.359	0.00	73.10	B
	ATOM	2996	CD	GLU	B	518	90.441	-11.970	58.079	0.00	73.51	B
30	ATOM	2997	OE1	GLU	B	518	89.258	-12.335	58.243	0.00	73.72	B
	ATOM	2998	OE2	GLU	B	518	91.346	-12.741	57.695	0.00	73.72	B
	ATOM	2999	C	GLU	B	518	90.145	-7.730	59.199	1.00	70.28	B
	ATOM	3000	O	GLU	B	518	90.596	-7.400	58.098	1.00	69.72	B
	ATOM	3001	N	ASN	B	519	88.977	-7.296	59.676	1.00	68.04	B
35	ATOM	3002	CA	ASN	B	519	88.087	-6.380	58.947	1.00	65.05	B
	ATOM	3003	CB	ASN	B	519	86.773	-6.224	59.718	1.00	63.79	B
	ATOM	3004	CG	ASN	B	519	85.805	-5.267	59.053	1.00	62.26	B
	ATOM	3005	OD1	ASN	B	519	84.702	-5.066	59.548	1.00	62.79	B
	ATOM	3006	ND2	ASN	B	519	86.204	-4.676	57.933	1.00	60.05	B
40	ATOM	3007	C	ASN	B	519	88.716	-5.000	58.728	1.00	63.93	B
	ATOM	3008	O	ASN	B	519	88.842	-4.220	59.669	1.00	64.23	B
	ATOM	3009	N	PRO	B	520	89.090	-4.673	57.473	1.00	62.40	B
	ATOM	3010	CD	PRO	B	520	88.866	-5.499	56.274	1.00	61.90	B
	ATOM	3011	CA	PRO	B	520	89.711	-3.396	57.096	1.00	60.68	B
45	ATOM	3012	CB	PRO	B	520	89.820	-3.497	55.577	1.00	60.59	B
	ATOM	3013	CG	PRO	B	520	89.895	-4.957	55.331	1.00	61.94	B
	ATOM	3014	C	PRO	B	520	88.906	-2.174	57.500	1.00	60.35	B
	ATOM	3015	O	PRO	B	520	89.403	-1.049	57.445	1.00	60.91	B
	ATOM	3016	N	TYR	B	521	87.657	-2.399	57.888	1.00	58.53	B
50	ATOM	3017	CA	TYR	B	521	86.774	-1.314	58.276	1.00	56.62	B
	ATOM	3018	CB	TYR	B	521	85.410	-1.538	57.636	1.00	56.52	B
	ATOM	3019	CG	TYR	B	521	85.470	-1.631	56.133	1.00	55.43	B
	ATOM	3020	CD1	TYR	B	521	85.625	-0.493	55.356	1.00	53.35	B
	ATOM	3021	CE1	TYR	B	521	85.684	-0.568	53.980	1.00	52.25	B

	ATOM	3022	CD2	TYR	B	521	85.378	-2.860	55.487	1.00	55.47	B
	ATOM	3023	CE2	TYR	B	521	85.437	-2.946	54.109	1.00	54.04	B
	ATOM	3024	CZ	TYR	B	521	85.587	-1.792	53.360	1.00	53.20	B
	ATOM	3025	OH	TYR	B	521	85.611	-1.862	51.986	1.00	53.19	B
5	ATOM	3026	C	TYR	B	521	86.618	-1.168	59.782	1.00	56.07	B
	ATOM	3027	O	TYR	B	521	86.225	-0.109	60.264	1.00	55.68	B
	ATOM	3028	N	PHE	B	522	86.929	-2.227	60.521	1.00	55.73	B
	ATOM	3029	CA	PHE	B	522	86.797	-2.207	61.969	1.00	55.79	B
	ATOM	3030	CB	PHE	B	522	86.993	-3.605	62.543	1.00	57.01	B
10	ATOM	3031	CG	PHE	B	522	86.935	-3.654	64.046	1.00	59.45	B
	ATOM	3032	CD1	PHE	B	522	85.730	-3.458	64.719	1.00	60.43	B
	ATOM	3033	CD2	PHE	B	522	88.084	-3.895	64.794	1.00	59.23	B
	ATOM	3034	CE1	PHE	B	522	85.672	-3.505	66.119	1.00	60.50	B
	ATOM	3035	CE2	PHE	B	522	88.032	-3.943	66.192	1.00	59.21	B
15	ATOM	3036	CZ	PHE	B	522	86.825	-3.749	66.856	1.00	58.74	B
	ATOM	3037	C	PHE	B	522	87.764	-1.267	62.668	1.00	55.79	B
	ATOM	3038	O	PHE	B	522	88.899	-1.643	62.962	1.00	56.44	B
	ATOM	3039	N	VAL	B	523	87.314	-0.048	62.951	1.00	56.06	B
	ATOM	3040	CA	VAL	B	523	88.155	0.924	63.650	1.00	55.15	B
20	ATOM	3041	CB	VAL	B	523	87.445	2.271	63.817	1.00	53.14	B
	ATOM	3042	CG1	VAL	B	523	88.324	3.223	64.601	1.00	51.48	B
	ATOM	3043	CG2	VAL	B	523	87.113	2.844	62.460	1.00	53.68	B
	ATOM	3044	C	VAL	B	523	88.506	0.384	65.035	1.00	55.15	B
	ATOM	3045	O	VAL	B	523	89.675	0.140	65.331	1.00	55.89	B
25	ATOM	3046	N	GLY	B	524	87.489	0.187	65.870	1.00	53.67	B
	ATOM	3047	CA	GLY	B	524	87.726	-0.325	67.205	1.00	52.15	B
	ATOM	3048	C	GLY	B	524	86.521	-0.286	68.127	1.00	50.48	B
	ATOM	3049	O	GLY	B	524	85.504	0.329	67.821	1.00	50.52	B
	ATOM	3050	N	VAL	B	525	86.643	-0.933	69.277	1.00	48.79	B
30	ATOM	3051	CA	VAL	B	525	85.555	-0.975	70.232	1.00	48.07	B
	ATOM	3052	CB	VAL	B	525	85.354	-2.418	70.744	1.00	46.89	B
	ATOM	3053	CG1	VAL	B	525	86.674	-3.138	70.750	1.00	45.99	B
	ATOM	3054	CG2	VAL	B	525	84.732	-2.403	72.130	1.00	45.90	B
	ATOM	3055	C	VAL	B	525	85.800	-0.015	71.392	1.00	47.57	B
35	ATOM	3056	O	VAL	B	525	86.938	0.175	71.805	1.00	46.79	B
	ATOM	3057	N	LEU	B	526	84.727	0.603	71.894	1.00	48.52	B
	ATOM	3058	CA	LEU	B	526	84.811	1.567	73.005	1.00	48.97	B
	ATOM	3059	CB	LEU	B	526	84.199	2.910	72.583	1.00	47.57	B
	ATOM	3060	CG	LEU	B	526	84.696	3.601	71.310	1.00	47.85	B
40	ATOM	3061	CD1	LEU	B	526	83.713	4.694	70.936	1.00	48.90	B
	ATOM	3062	CD2	LEU	B	526	86.082	4.170	71.496	1.00	46.34	B
	ATOM	3063	C	LEU	B	526	84.078	1.047	74.257	1.00	49.07	B
	ATOM	3064	O	LEU	B	526	82.862	1.207	74.382	1.00	49.55	B
	ATOM	3065	N	ARG	B	527	84.820	0.425	75.174	1.00	48.77	B
45	ATOM	3066	CA	ARG	B	527	84.239	-0.119	76.402	1.00	48.18	B
	ATOM	3067	CB	ARG	B	527	85.016	-1.349	76.877	1.00	47.43	B
	ATOM	3068	CG	ARG	B	527	84.725	-2.604	76.074	1.00	47.62	B
	ATOM	3069	CD	ARG	B	527	85.540	-3.794	76.557	1.00	45.88	B
	ATOM	3070	NE	ARG	B	527	86.528	-4.196	75.561	1.00	44.94	B
50	ATOM	3071	CZ	ARG	B	527	86.259	-4.860	74.439	1.00	43.61	B
	ATOM	3072	NH1	ARG	B	527	85.014	-5.218	74.152	1.00	41.64	B
	ATOM	3073	NH2	ARG	B	527	87.246	-5.158	73.594	1.00	41.55	B
	ATOM	3074	C	ARG	B	527	84.214	0.907	77.515	1.00	47.73	B
	ATOM	3075	O	ARG	B	527	85.162	1.662	77.703	1.00	46.73	B

	ATOM	3076	N	GLY	B	528	83.120	0.929	78.259	1.00	48.05	B
	ATOM	3077	CA	GLY	B	528	83.013	1.888	79.338	1.00	49.61	B
	ATOM	3078	C	GLY	B	528	81.677	1.823	80.047	1.00	50.20	B
5	ATOM	3079	O	GLY	B	528	81.510	2.397	81.120	1.00	50.44	B
	ATOM	3080	N	HIS	B	529	80.718	1.126	79.448	1.00	51.40	B
	ATOM	3081	CA	HIS	B	529	79.392	0.990	80.040	1.00	52.69	B
	ATOM	3082	CB	HIS	B	529	78.308	1.270	78.997	1.00	53.42	B
	ATOM	3083	CG	HIS	B	529	77.908	2.711	78.931	1.00	54.66	B
10	ATOM	3084	CD2	HIS	B	529	78.036	3.710	79.836	1.00	54.96	B
	ATOM	3085	ND1	HIS	B	529	77.284	3.264	77.835	1.00	54.53	B
	ATOM	3086	CE1	HIS	B	529	77.046	4.542	78.066	1.00	54.69	B
	ATOM	3087	NE2	HIS	B	529	77.493	4.837	79.273	1.00	55.98	B
	ATOM	3088	C	HIS	B	529	79.174	-0.376	80.664	1.00	52.47	B
15	ATOM	3089	O	HIS	B	529	79.576	-1.396	80.112	1.00	53.72	B
	ATOM	3090	N	MSE	B	530	78.531	-0.379	81.825	1.00	52.35	B
	ATOM	3091	CA	MSE	B	530	78.260	-1.603	82.568	1.00	51.79	B
	ATOM	3092	CB	MSE	B	530	78.325	-1.325	84.068	1.00	54.89	B
	ATOM	3093	CG	MSE	B	530	79.640	-0.727	84.520	1.00	59.05	B
20	ATOM	3094	SE	MSE	B	530	81.160	-1.831	84.066	1.00	66.13	B
	ATOM	3095	CE	MSE	B	530	81.008	-3.077	85.560	1.00	62.20	B
	ATOM	3096	C	MSE	B	530	76.894	-2.153	82.241	1.00	50.13	B
	ATOM	3097	O	MSE	B	530	76.318	-2.887	83.036	1.00	49.11	B
	ATOM	3098	N	ALA	B	531	76.379	-1.800	81.070	1.00	49.94	B
25	ATOM	3099	CA	ALA	B	531	75.055	-2.246	80.658	1.00	48.69	B
	ATOM	3100	CB	ALA	B	531	73.999	-1.553	81.498	1.00	48.43	B
	ATOM	3101	C	ALA	B	531	74.843	-1.928	79.189	1.00	47.77	B
	ATOM	3102	O	ALA	B	531	75.669	-1.256	78.566	1.00	48.05	B
	ATOM	3103	N	SER	B	532	73.731	-2.414	78.645	1.00	46.82	B
30	ATOM	3104	CA	SER	B	532	73.380	-2.196	77.242	1.00	45.70	B
	ATOM	3105	CB	SER	B	532	72.036	-2.855	76.921	1.00	45.79	B
	ATOM	3106	OG	SER	B	532	71.413	-2.223	75.811	1.00	44.70	B
	ATOM	3107	C	SER	B	532	73.306	-0.733	76.839	1.00	44.93	B
	ATOM	3108	O	SER	B	532	72.834	0.118	77.595	1.00	45.32	B
35	ATOM	3109	N	VAL	B	533	73.775	-0.469	75.627	1.00	43.79	B
	ATOM	3110	CA	VAL	B	533	73.771	0.865	75.038	1.00	43.92	B
	ATOM	3111	CB	VAL	B	533	75.002	1.045	74.123	1.00	42.68	B
	ATOM	3112	CG1	VAL	B	533	74.893	2.335	73.336	1.00	42.48	B
	ATOM	3113	CG2	VAL	B	533	76.274	1.027	74.965	1.00	41.21	B
40	ATOM	3114	C	VAL	B	533	72.480	1.013	74.215	1.00	43.88	B
	ATOM	3115	O	VAL	B	533	72.398	0.518	73.085	1.00	43.85	B
	ATOM	3116	N	ARG	B	534	71.479	1.689	74.787	1.00	42.61	B
	ATOM	3117	CA	ARG	B	534	70.174	1.867	74.136	1.00	40.98	B
	ATOM	3118	CB	ARG	B	534	69.074	2.081	75.177	1.00	41.23	B
45	ATOM	3119	CG	ARG	B	534	67.896	1.146	75.017	1.00	42.21	B
	ATOM	3120	CD	ARG	B	534	66.586	1.862	74.752	1.00	43.49	B
	ATOM	3121	NE	ARG	B	534	66.301	2.077	73.331	1.00	45.72	B
	ATOM	3122	CZ	ARG	B	534	65.097	1.903	72.792	1.00	47.54	B
	ATOM	3123	NH1	ARG	B	534	64.093	1.508	73.563	1.00	46.82	B
50	ATOM	3124	NH2	ARG	B	534	64.884	2.136	71.499	1.00	50.38	B
	ATOM	3125	C	ARG	B	534	70.104	3.015	73.162	1.00	39.36	B
	ATOM	3126	O	ARG	B	534	69.339	2.975	72.200	1.00	38.05	B
	ATOM	3127	N	THR	B	535	70.889	4.050	73.426	1.00	38.74	B
	ATOM	3128	CA	THR	B	535	70.869	5.217	72.566	1.00	38.25	B
	ATOM	3129	CB	THR	B	535	70.062	6.362	73.233	1.00	39.86	B

	ATOM	3130	OG1	THR	B	535	70.130	7.534	72.411	1.00	42.15	B
	ATOM	3131	CG2	THR	B	535	70.596	6.661	74.630	1.00	39.79	B
	ATOM	3132	C	THR	B	535	72.263	5.686	72.189	1.00	36.40	B
	ATOM	3133	O	THR	B	535	73.212	5.478	72.934	1.00	34.48	B
5	ATOM	3134	N	VAL	B	536	72.369	6.300	71.013	1.00	36.97	B
	ATOM	3135	CA	VAL	B	536	73.637	6.798	70.482	1.00	38.48	B
	ATOM	3136	CB	VAL	B	536	74.365	5.725	69.663	1.00	39.79	B
	ATOM	3137	CG1	VAL	B	536	75.570	6.344	68.958	1.00	39.98	B
	ATOM	3138	CG2	VAL	B	536	74.807	4.588	70.561	1.00	42.70	B
10	ATOM	3139	C	VAL	B	536	73.417	7.969	69.538	1.00	37.98	B
	ATOM	3140	O	VAL	B	536	72.705	7.836	68.544	1.00	39.94	B
	ATOM	3141	N	SER	B	537	74.037	9.105	69.832	1.00	36.75	B
	ATOM	3142	CA	SER	B	537	73.904	10.281	68.978	1.00	35.47	B
	ATOM	3143	CB	SER	B	537	72.974	11.296	69.646	1.00	36.17	B
15	ATOM	3144	OG	SER	B	537	73.057	12.572	69.032	1.00	36.43	B
	ATOM	3145	C	SER	B	537	75.280	10.889	68.744	1.00	34.85	B
	ATOM	3146	O	SER	B	537	76.071	11.009	69.671	1.00	33.64	B
	ATOM	3147	N	GLY	B	538	75.575	11.258	67.507	1.00	34.65	B
	ATOM	3148	CA	GLY	B	538	76.875	11.836	67.243	1.00	37.80	B
20	ATOM	3149	C	GLY	B	538	76.900	12.740	66.030	1.00	39.65	B
	ATOM	3150	O	GLY	B	538	75.937	12.783	65.270	1.00	39.10	B
	ATOM	3151	N	HIS	B	539	78.004	13.462	65.857	1.00	42.51	B
	ATOM	3152	CA	HIS	B	539	78.193	14.382	64.736	1.00	44.95	B
	ATOM	3153	CB	HIS	B	539	77.370	15.657	64.927	1.00	48.76	B
25	ATOM	3154	CG	HIS	B	539	75.912	15.402	65.134	1.00	54.64	B
	ATOM	3155	CD2	HIS	B	539	75.121	15.566	66.221	1.00	55.81	B
	ATOM	3156	ND1	HIS	B	539	75.112	14.845	64.158	1.00	55.89	B
	ATOM	3157	CE1	HIS	B	539	73.891	14.677	64.635	1.00	56.19	B
	ATOM	3158	NE2	HIS	B	539	73.870	15.106	65.885	1.00	56.92	B
30	ATOM	3159	C	HIS	B	539	79.665	14.753	64.709	1.00	45.08	B
	ATOM	3160	O	HIS	B	539	80.167	15.351	65.659	1.00	45.61	B
	ATOM	3161	N	GLY	B	540	80.357	14.409	63.627	1.00	44.60	B
	ATOM	3162	CA	GLY	B	540	81.773	14.727	63.538	1.00	44.51	B
	ATOM	3163	C	GLY	B	540	82.612	13.714	64.300	1.00	44.45	B
35	ATOM	3164	O	GLY	B	540	82.356	12.519	64.188	1.00	44.43	B
	ATOM	3165	N	ASN	B	541	83.612	14.182	65.054	1.00	44.24	B
	ATOM	3166	CA	ASN	B	541	84.482	13.304	65.841	1.00	43.77	B
	ATOM	3167	CB	ASN	B	541	85.914	13.855	65.925	1.00	43.91	B
	ATOM	3168	CG	ASN	B	541	86.011	15.119	66.773	1.00	45.62	B
40	ATOM	3169	OD1	ASN	B	541	85.399	16.139	66.449	1.00	46.42	B
	ATOM	3170	ND2	ASN	B	541	86.783	15.054	67.867	1.00	45.00	B
	ATOM	3171	C	ASN	B	541	83.949	13.134	67.257	1.00	43.38	B
	ATOM	3172	O	ASN	B	541	84.662	12.651	68.139	1.00	44.20	B
	ATOM	3173	N	ILE	B	542	82.697	13.530	67.475	1.00	41.65	B
45	ATOM	3174	CA	ILE	B	542	82.067	13.418	68.789	1.00	40.51	B
	ATOM	3175	CB	ILE	B	542	81.681	14.821	69.350	1.00	41.10	B
	ATOM	3176	CG2	ILE	B	542	81.158	14.690	70.779	1.00	39.51	B
	ATOM	3177	CG1	ILE	B	542	82.893	15.753	69.325	1.00	39.00	B
	ATOM	3178	CD1	ILE	B	542	84.043	15.278	70.192	1.00	38.09	B
50	ATOM	3179	C	ILE	B	542	80.795	12.560	68.744	1.00	39.78	B
	ATOM	3180	O	ILE	B	542	79.939	12.740	67.870	1.00	38.52	B
	ATOM	3181	N	VAL	B	543	80.687	11.630	69.691	1.00	38.75	B
	ATOM	3182	CA	VAL	B	543	79.523	10.752	69.799	1.00	38.25	B
	ATOM	3183	CB	VAL	B	543	79.775	9.342	69.183	1.00	37.58	B

	ATOM	3184	CG1	VAL	B	543	78.596	8.430	69.454	1.00	34.60	B
	ATOM	3185	CG2	VAL	B	543	79.995	9.459	67.678	1.00	39.64	B
	ATOM	3186	C	VAL	B	543	79.198	10.573	71.270	1.00	37.91	B
	ATOM	3187	O	VAL	B	543	80.098	10.411	72.091	1.00	40.30	B
5	ATOM	3188	N	VAL	B	544	77.913	10.602	71.605	1.00	35.82	B
	ATOM	3189	CA	VAL	B	544	77.490	10.435	72.985	1.00	32.38	B
	ATOM	3190	CB	VAL	B	544	76.637	11.600	73.437	1.00	31.34	B
	ATOM	3191	CG1	VAL	B	544	76.364	11.471	74.913	1.00	31.93	B
	ATOM	3192	CG2	VAL	B	544	77.321	12.904	73.104	1.00	30.92	B
10	ATOM	3193	C	VAL	B	544	76.652	9.186	73.089	1.00	31.39	B
	ATOM	3194	O	VAL	B	544	75.764	8.976	72.279	1.00	32.39	B
	ATOM	3195	N	SER	B	545	76.913	8.359	74.089	1.00	31.37	B
	ATOM	3196	CA	SER	B	545	76.136	7.135	74.238	1.00	32.82	B
	ATOM	3197	CB	SER	B	545	77.067	5.911	74.166	1.00	33.04	B
15	ATOM	3198	OG	SER	B	545	77.887	5.768	75.328	1.00	31.94	B
	ATOM	3199	C	SER	B	545	75.290	7.062	75.522	1.00	34.31	B
	ATOM	3200	O	SER	B	545	75.663	7.595	76.576	1.00	35.23	B
	ATOM	3201	N	GLY	B	546	74.157	6.373	75.421	1.00	35.10	B
	ATOM	3202	CA	GLY	B	546	73.271	6.209	76.558	1.00	35.16	B
20	ATOM	3203	C	GLY	B	546	73.064	4.744	76.889	1.00	35.12	B
	ATOM	3204	O	GLY	B	546	72.627	3.952	76.048	1.00	36.06	B
	ATOM	3205	N	SER	B	547	73.370	4.377	78.122	1.00	34.92	B
	ATOM	3206	CA	SER	B	547	73.219	2.996	78.520	1.00	35.83	B
	ATOM	3207	CB	SER	B	547	74.542	2.450	79.054	1.00	36.42	B
25	ATOM	3208	OG	SER	B	547	74.376	1.145	79.580	1.00	37.41	B
	ATOM	3209	C	SER	B	547	72.146	2.811	79.569	1.00	36.27	B
	ATOM	3210	O	SER	B	547	71.561	3.776	80.043	1.00	35.05	B
	ATOM	3211	N	TYR	B	548	71.881	1.555	79.908	1.00	38.32	B
	ATOM	3212	CA	TYR	B	548	70.890	1.227	80.916	1.00	40.30	B
30	ATOM	3213	CB	TYR	B	548	70.288	-0.146	80.629	1.00	42.68	B
	ATOM	3214	CG	TYR	B	548	69.117	-0.134	79.670	1.00	45.80	B
	ATOM	3215	CD1	TYR	B	548	68.593	1.068	79.174	1.00	47.24	B
	ATOM	3216	CE1	TYR	B	548	67.472	1.074	78.345	1.00	47.96	B
	ATOM	3217	CD2	TYR	B	548	68.494	-1.322	79.302	1.00	45.36	B
35	ATOM	3218	CE2	TYR	B	548	67.385	-1.325	78.481	1.00	46.33	B
	ATOM	3219	CZ	TYR	B	548	66.873	-0.135	78.008	1.00	47.54	B
	ATOM	3220	OH	TYR	B	548	65.744	-0.162	77.223	1.00	49.19	B
	ATOM	3221	C	TYR	B	548	71.550	1.228	82.289	1.00	40.55	B
	ATOM	3222	O	TYR	B	548	70.898	0.990	83.305	1.00	40.82	B
40	ATOM	3223	N	ASP	B	549	72.852	1.496	82.315	1.00	40.33	B
	ATOM	3224	CA	ASP	B	549	73.574	1.523	83.572	1.00	40.21	B
	ATOM	3225	CB	ASP	B	549	75.053	1.177	83.352	1.00	38.64	B
	ATOM	3226	CG	ASP	B	549	75.813	2.287	82.659	1.00	39.21	B
	ATOM	3227	OD1	ASP	B	549	75.195	3.348	82.399	1.00	39.42	B
45	ATOM	3228	OD2	ASP	B	549	77.025	2.106	82.389	1.00	35.60	B
	ATOM	3229	C	ASP	B	549	73.437	2.905	84.207	1.00	41.08	B
	ATOM	3230	O	ASP	B	549	74.180	3.251	85.125	1.00	41.91	B
	ATOM	3231	N	ASN	B	550	72.490	3.693	83.696	1.00	41.46	B
	ATOM	3232	CA	ASN	B	550	72.213	5.043	84.208	1.00	41.90	B
50	ATOM	3233	CB	ASN	B	550	71.853	4.982	85.696	1.00	42.29	B
	ATOM	3234	CG	ASN	B	550	70.885	3.882	86.013	1.00	42.40	B
	ATOM	3235	OD1	ASN	B	550	70.421	3.181	85.117	1.00	44.98	B
	ATOM	3236	ND2	ASN	B	550	70.563	3.723	87.289	1.00	41.54	B
	ATOM	3237	C	ASN	B	550	73.430	5.944	84.049	1.00	41.35	B

	ATOM	3238	O	ASN	B	550	73.934	6.498	85.034	1.00	41.70	B
	ATOM	3239	N	THR	B	551	73.891	6.101	82.816	1.00	40.29	B
	ATOM	3240	CA	THR	B	551	75.081	6.890	82.562	1.00	40.46	B
	ATOM	3241	CB	THR	B	551	76.344	6.109	83.031	1.00	40.37	B
5	ATOM	3242	OG1	THR	B	551	76.524	6.278	84.437	1.00	40.39	B
	ATOM	3243	CG2	THR	B	551	77.576	6.547	82.288	1.00	39.19	B
	ATOM	3244	C	THR	B	551	75.230	7.167	81.080	1.00	41.05	B
	ATOM	3245	O	THR	B	551	74.793	6.374	80.250	1.00	41.68	B
	ATOM	3246	N	LEU	B	552	75.849	8.295	80.754	1.00	40.71	B
10	ATOM	3247	CA	LEU	B	552	76.098	8.659	79.368	1.00	40.16	B
	ATOM	3248	CB	LEU	B	552	75.354	9.943	78.994	1.00	39.03	B
	ATOM	3249	CG	LEU	B	552	73.828	9.882	78.968	1.00	38.53	B
	ATOM	3250	CD1	LEU	B	552	73.257	10.693	80.130	1.00	38.23	B
	ATOM	3251	CD2	LEU	B	552	73.327	10.416	77.631	1.00	37.33	B
15	ATOM	3252	C	LEU	B	552	77.591	8.888	79.253	1.00	40.99	B
	ATOM	3253	O	LEU	B	552	78.225	9.325	80.213	1.00	41.44	B
	ATOM	3254	N	ILE	B	553	78.160	8.579	78.093	1.00	41.46	B
	ATOM	3255	CA	ILE	B	553	79.589	8.788	77.879	1.00	41.69	B
	ATOM	3256	CB	ILE	B	553	80.366	7.452	77.679	1.00	41.75	B
20	ATOM	3257	CG2	ILE	B	553	81.854	7.746	77.598	1.00	41.32	B
	ATOM	3258	CG1	ILE	B	553	80.077	6.451	78.811	1.00	42.93	B
	ATOM	3259	CD1	ILE	B	553	80.616	6.835	80.176	1.00	42.43	B
	ATOM	3260	C	ILE	B	553	79.774	9.615	76.612	1.00	41.85	B
	ATOM	3261	O	ILE	B	553	79.057	9.419	75.631	1.00	41.17	B
25	ATOM	3262	N	VAL	B	554	80.724	10.547	76.638	1.00	42.67	B
	ATOM	3263	CA	VAL	B	554	81.022	11.371	75.467	1.00	43.83	B
	ATOM	3264	CB	VAL	B	554	81.216	12.850	75.832	1.00	43.23	B
	ATOM	3265	CG1	VAL	B	554	81.219	13.690	74.566	1.00	41.99	B
	ATOM	3266	CG2	VAL	B	554	80.143	13.294	76.799	1.00	43.78	B
30	ATOM	3267	C	VAL	B	554	82.344	10.858	74.907	1.00	44.98	B
	ATOM	3268	O	VAL	B	554	83.391	11.108	75.489	1.00	45.12	B
	ATOM	3269	N	TRP	B	555	82.305	10.152	73.782	1.00	46.53	B
	ATOM	3270	CA	TRP	B	555	83.526	9.603	73.198	1.00	48.33	B
	ATOM	3271	CB	TRP	B	555	83.264	8.193	72.652	1.00	48.73	B
35	ATOM	3272	CG	TRP	B	555	82.491	7.287	73.562	1.00	48.42	B
	ATOM	3273	CD2	TRP	B	555	83.024	6.244	74.390	1.00	49.05	B
	ATOM	3274	CE2	TRP	B	555	81.934	5.644	75.060	1.00	49.51	B
	ATOM	3275	CE3	TRP	B	555	84.317	5.758	74.629	1.00	48.35	B
	ATOM	3276	CD1	TRP	B	555	81.140	7.281	73.762	1.00	48.53	B
40	ATOM	3277	NE1	TRP	B	555	80.797	6.296	74.661	1.00	49.31	B
	ATOM	3278	CZ2	TRP	B	555	82.099	4.579	75.958	1.00	49.91	B
	ATOM	3279	CZ3	TRP	B	555	84.481	4.698	75.523	1.00	47.73	B
	ATOM	3280	CH2	TRP	B	555	83.378	4.121	76.174	1.00	48.67	B
	ATOM	3281	C	TRP	B	555	84.119	10.455	72.074	1.00	49.09	B
45	ATOM	3282	O	TRP	B	555	83.424	11.253	71.451	1.00	48.46	B
	ATOM	3283	N	ASP	B	556	85.411	10.265	71.816	1.00	51.15	B
	ATOM	3284	CA	ASP	B	556	86.119	10.978	70.745	1.00	52.97	B
	ATOM	3285	CB	ASP	B	556	87.358	11.705	71.295	1.00	53.47	B
	ATOM	3286	CG	ASP	B	556	88.047	12.594	70.247	1.00	53.63	B
50	ATOM	3287	OD1	ASP	B	556	88.097	12.203	69.060	1.00	52.44	B
	ATOM	3288	OD2	ASP	B	556	88.552	13.683	70.615	1.00	53.83	B
	ATOM	3289	C	ASP	B	556	86.569	9.933	69.726	1.00	53.38	B
	ATOM	3290	O	ASP	B	556	87.740	9.560	69.688	1.00	54.18	B
	ATOM	3291	N	VAL	B	557	85.635	9.460	68.909	1.00	54.03	B

	ATOM	3292	CA	VAL	B	557	85.925	8.446	67.896	1.00	53.93	B
	ATOM	3293	CB	VAL	B	557	84.859	8.493	66.780	1.00	53.70	B
	ATOM	3294	CG1	VAL	B	557	85.210	7.519	65.660	1.00	54.83	B
	ATOM	3295	CG2	VAL	B	557	83.502	8.151	67.370	1.00	52.75	B
5	ATOM	3296	C	VAL	B	557	87.327	8.578	67.295	1.00	54.01	B
	ATOM	3297	O	VAL	B	557	88.014	7.575	67.065	1.00	53.12	B
	ATOM	3298	N	ALA	B	558	87.752	9.817	67.063	1.00	54.57	B
	ATOM	3299	CA	ALA	B	558	89.071	10.087	66.497	1.00	55.27	B
	ATOM	3300	CB	ALA	B	558	89.249	11.577	66.286	1.00	54.44	B
10	ATOM	3301	C	ALA	B	558	90.189	9.554	67.393	1.00	56.09	B
	ATOM	3302	O	ALA	B	558	91.154	8.948	66.917	1.00	57.14	B
	ATOM	3303	N	GLN	B	559	90.054	9.779	68.693	1.00	56.27	B
	ATOM	3304	CA	GLN	B	559	91.052	9.325	69.652	1.00	56.00	B
	ATOM	3305	CB	GLN	B	559	91.358	10.445	70.643	1.00	57.58	B
15	ATOM	3306	CG	GLN	B	559	91.679	11.771	69.977	1.00	60.76	B
	ATOM	3307	CD	GLN	B	559	92.288	12.773	70.944	1.00	63.21	B
	ATOM	3308	OE1	GLN	B	559	91.798	12.942	72.072	1.00	63.29	B
	ATOM	3309	NE2	GLN	B	559	93.360	13.449	70.510	1.00	62.95	B
	ATOM	3310	C	GLN	B	559	90.556	8.090	70.400	1.00	54.82	B
20	ATOM	3311	O	GLN	B	559	91.131	7.679	71.407	1.00	53.08	B
	ATOM	3312	N	MSE	B	560	89.486	7.500	69.885	1.00	54.44	B
	ATOM	3313	CA	MSE	B	560	88.881	6.322	70.487	1.00	54.74	B
	ATOM	3314	CB	MSE	B	560	89.450	5.055	69.844	1.00	54.65	B
	ATOM	3315	CG	MSE	B	560	89.124	4.912	68.360	1.00	54.73	B
25	ATOM	3316	SE	MSE	B	560	87.225	4.845	67.991	1.00	57.83	B
	ATOM	3317	CE	MSE	B	560	86.882	2.985	68.379	1.00	53.96	B
	ATOM	3318	C	MSE	B	560	89.041	6.275	72.013	1.00	54.33	B
	ATOM	3319	O	MSE	B	560	89.330	5.230	72.600	1.00	54.09	B
	ATOM	3320	N	LYS	B	561	88.838	7.419	72.654	1.00	53.76	B
30	ATOM	3321	CA	LYS	B	561	88.945	7.494	74.100	1.00	53.03	B
	ATOM	3322	CB	LYS	B	561	90.168	8.331	74.473	0.00	53.61	B
	ATOM	3323	CG	LYS	B	561	90.538	8.294	75.933	0.00	54.07	B
	ATOM	3324	CD	LYS	B	561	91.867	8.981	76.146	0.00	54.52	B
	ATOM	3325	CE	LYS	B	561	92.219	9.039	77.612	0.00	54.82	B
35	ATOM	3326	NZ	LYS	B	561	91.225	9.852	78.361	0.00	55.11	B
	ATOM	3327	C	LYS	B	561	87.663	8.092	74.690	1.00	52.48	B
	ATOM	3328	O	LYS	B	561	86.786	8.548	73.952	1.00	53.43	B
	ATOM	3329	N	CYS	B	562	87.553	8.063	76.018	1.00	50.98	B
	ATOM	3330	CA	CYS	B	562	86.394	8.601	76.740	1.00	48.94	B
40	ATOM	3331	CB	CYS	B	562	86.209	7.834	78.056	1.00	49.61	B
	ATOM	3332	SG	CYS	B	562	85.037	8.536	79.259	1.00	51.47	B
	ATOM	3333	C	CYS	B	562	86.646	10.076	77.029	1.00	47.64	B
	ATOM	3334	O	CYS	B	562	87.772	10.450	77.339	1.00	48.22	B
	ATOM	3335	N	LEU	B	563	85.616	10.915	76.909	1.00	46.12	B
45	ATOM	3336	CA	LEU	B	563	85.771	12.346	77.175	1.00	44.98	B
	ATOM	3337	CB	LEU	B	563	85.149	13.187	76.051	1.00	44.96	B
	ATOM	3338	CG	LEU	B	563	85.894	13.179	74.706	1.00	46.73	B
	ATOM	3339	CD1	LEU	B	563	85.234	14.142	73.721	1.00	45.90	B
	ATOM	3340	CD2	LEU	B	563	87.346	13.583	74.931	1.00	45.81	B
50	ATOM	3341	C	LEU	B	563	85.165	12.731	78.518	1.00	43.88	B
	ATOM	3342	O	LEU	B	563	85.823	13.367	79.348	1.00	43.62	B
	ATOM	3343	N	TYR	B	564	83.913	12.345	78.731	1.00	42.63	B
	ATOM	3344	CA	TYR	B	564	83.244	12.632	79.986	1.00	41.64	B
	ATOM	3345	CB	TYR	B	564	82.429	13.918	79.887	1.00	41.63	B

	ATOM	3346	CG	TYR	B	564	83.248	15.149	79.592	1.00	42.86	B
	ATOM	3347	CD1	TYR	B	564	83.298	15.684	78.308	1.00	43.33	B
	ATOM	3348	CE1	TYR	B	564	84.049	16.819	78.036	1.00	45.08	B
	ATOM	3349	CD2	TYR	B	564	83.976	15.782	80.602	1.00	43.76	B
5	ATOM	3350	CE2	TYR	B	564	84.732	16.916	80.341	1.00	43.78	B
	ATOM	3351	CZ	TYR	B	564	84.760	17.426	79.060	1.00	46.05	B
	ATOM	3352	OH	TYR	B	564	85.492	18.558	78.795	1.00	48.58	B
	ATOM	3353	C	TYR	B	564	82.321	11.491	80.356	1.00	41.77	B
	ATOM	3354	O	TYR	B	564	81.899	10.722	79.489	1.00	42.27	B
10	ATOM	3355	N	ILE	B	565	82.011	11.391	81.647	1.00	41.33	B
	ATOM	3356	CA	ILE	B	565	81.116	10.358	82.156	1.00	40.82	B
	ATOM	3357	CB	ILE	B	565	81.828	9.414	83.169	1.00	41.48	B
	ATOM	3358	CG2	ILE	B	565	80.934	8.234	83.486	1.00	40.38	B
	ATOM	3359	CG1	ILE	B	565	83.126	8.862	82.582	1.00	40.59	B
15	ATOM	3360	CD1	ILE	B	565	83.907	8.008	83.571	1.00	41.08	B
	ATOM	3361	C	ILE	B	565	79.938	11.020	82.860	1.00	40.09	B
	ATOM	3362	O	ILE	B	565	79.853	11.020	84.089	1.00	41.84	B
	ATOM	3363	N	LEU	B	566	79.033	11.582	82.067	1.00	38.80	B
	ATOM	3364	CA	LEU	B	566	77.841	12.256	82.580	1.00	36.98	B
20	ATOM	3365	CB	LEU	B	566	76.990	12.754	81.421	1.00	36.01	B
	ATOM	3366	CG	LEU	B	566	77.792	13.369	80.272	1.00	35.51	B
	ATOM	3367	CD1	LEU	B	566	76.846	13.709	79.138	1.00	34.67	B
	ATOM	3368	CD2	LEU	B	566	78.541	14.592	80.757	1.00	33.68	B
	ATOM	3369	C	LEU	B	566	77.010	11.306	83.411	1.00	36.96	B
25	ATOM	3370	O	LEU	B	566	76.354	10.414	82.877	1.00	36.93	B
	ATOM	3371	N	SER	B	567	77.021	11.498	84.721	1.00	37.95	B
	ATOM	3372	CA	SER	B	567	76.252	10.628	85.601	1.00	39.30	B
	ATOM	3373	CB	SER	B	567	77.191	9.655	86.305	1.00	39.73	B
	ATOM	3374	OG	SER	B	567	78.238	10.359	86.940	1.00	40.54	B
30	ATOM	3375	C	SER	B	567	75.466	11.417	86.635	1.00	39.56	B
	ATOM	3376	O	SER	B	567	76.007	12.260	87.344	1.00	39.82	B
	ATOM	3377	N	GLY	B	568	74.181	11.116	86.728	1.00	40.79	B
	ATOM	3378	CA	GLY	B	568	73.338	11.798	87.685	1.00	40.25	B
	ATOM	3379	C	GLY	B	568	71.949	11.190	87.704	1.00	40.41	B
35	ATOM	3380	O	GLY	B	568	71.270	11.232	88.723	1.00	41.14	B
	ATOM	3381	N	HIS	B	569	71.513	10.636	86.575	1.00	40.65	B
	ATOM	3382	CA	HIS	B	569	70.197	10.017	86.508	1.00	40.96	B
	ATOM	3383	CB	HIS	B	569	69.865	9.568	85.077	1.00	40.33	B
	ATOM	3384	CG	HIS	B	569	69.511	10.695	84.151	1.00	40.43	B
40	ATOM	3385	CD2	HIS	B	569	68.558	11.657	84.232	1.00	39.98	B
	ATOM	3386	ND1	HIS	B	569	70.194	10.936	82.977	1.00	40.06	B
	ATOM	3387	CE1	HIS	B	569	69.681	11.995	82.378	1.00	38.53	B
	ATOM	3388	NE2	HIS	B	569	68.687	12.452	83.118	1.00	38.90	B
	ATOM	3389	C	HIS	B	569	70.193	8.822	87.448	1.00	40.82	B
45	ATOM	3390	O	HIS	B	569	71.239	8.242	87.743	1.00	39.68	B
	ATOM	3391	N	THR	B	570	69.007	8.464	87.915	1.00	41.28	B
	ATOM	3392	CA	THR	B	570	68.857	7.364	88.838	1.00	41.75	B
	ATOM	3393	CB	THR	B	570	68.025	7.806	90.042	1.00	42.58	B
	ATOM	3394	OG1	THR	B	570	68.417	9.135	90.414	1.00	41.17	B
50	ATOM	3395	CG2	THR	B	570	68.265	6.872	91.226	1.00	44.09	B
	ATOM	3396	C	THR	B	570	68.201	6.169	88.168	1.00	41.63	B
	ATOM	3397	O	THR	B	570	67.554	5.348	88.824	1.00	42.87	B
	ATOM	3398	N	ASP	B	571	68.348	6.087	86.852	1.00	40.41	B
	ATOM	3399	CA	ASP	B	571	67.795	4.969	86.116	1.00	38.73	B

	ATOM	3400	CB	ASP	B	571	66.273	4.960	86.200	1.00	37.92	B
	ATOM	3401	CG	ASP	B	571	65.726	3.569	86.446	1.00	38.68	B
	ATOM	3402	OD1	ASP	B	571	66.270	2.616	85.852	1.00	37.31	B
	ATOM	3403	OD2	ASP	B	571	64.757	3.425	87.225	1.00	39.84	B
5	ATOM	3404	C	ASP	B	571	68.240	4.941	84.663	1.00	38.21	B
	ATOM	3405	O	ASP	B	571	68.800	5.914	84.147	1.00	37.05	B
	ATOM	3406	N	ARG	B	572	67.994	3.806	84.016	1.00	38.06	B
	ATOM	3407	CA	ARG	B	572	68.365	3.602	82.620	1.00	38.61	B
	ATOM	3408	CB	ARG	B	572	67.761	2.282	82.102	1.00	39.79	B
10	ATOM	3409	CG	ARG	B	572	66.409	1.944	82.735	1.00	42.08	B
	ATOM	3410	CD	ARG	B	572	65.669	0.771	82.066	1.00	43.20	B
	ATOM	3411	NE	ARG	B	572	66.402	-0.497	82.046	1.00	42.53	B
	ATOM	3412	CZ	ARG	B	572	65.859	-1.671	81.722	1.00	42.93	B
	ATOM	3413	NH1	ARG	B	572	64.573	-1.757	81.395	1.00	41.39	B
15	ATOM	3414	NH2	ARG	B	572	66.605	-2.764	81.708	1.00	43.19	B
	ATOM	3415	C	ARG	B	572	67.961	4.764	81.712	1.00	37.29	B
	ATOM	3416	O	ARG	B	572	66.923	5.408	81.911	1.00	37.19	B
	ATOM	3417	N	ILE	B	573	68.803	5.022	80.716	1.00	34.87	B
	ATOM	3418	CA	ILE	B	573	68.589	6.088	79.739	1.00	32.30	B
20	ATOM	3419	CB	ILE	B	573	69.914	6.783	79.417	1.00	31.72	B
	ATOM	3420	CG2	ILE	B	573	69.736	7.751	78.276	1.00	29.59	B
	ATOM	3421	CG1	ILE	B	573	70.434	7.465	80.678	1.00	33.36	B
	ATOM	3422	CD1	ILE	B	573	71.875	7.918	80.574	1.00	34.32	B
	ATOM	3423	C	ILE	B	573	68.024	5.489	78.454	1.00	30.51	B
25	ATOM	3424	O	ILE	B	573	68.467	4.441	78.009	1.00	29.57	B
	ATOM	3425	N	TYR	B	574	67.039	6.148	77.862	1.00	29.36	B
	ATOM	3426	CA	TYR	B	574	66.453	5.629	76.638	1.00	29.00	B
	ATOM	3427	CB	TYR	B	574	64.944	5.478	76.795	1.00	29.33	B
	ATOM	3428	CG	TYR	B	574	64.557	4.229	77.537	1.00	31.08	B
30	ATOM	3429	CD1	TYR	B	574	65.140	3.926	78.754	1.00	33.15	B
	ATOM	3430	CE1	TYR	B	574	64.782	2.797	79.465	1.00	33.55	B
	ATOM	3431	CD2	TYR	B	574	63.596	3.358	77.036	1.00	32.28	B
	ATOM	3432	CE2	TYR	B	574	63.225	2.209	77.748	1.00	32.21	B
	ATOM	3433	CZ	TYR	B	574	63.828	1.947	78.970	1.00	32.73	B
35	ATOM	3434	OH	TYR	B	574	63.457	0.871	79.743	1.00	34.36	B
	ATOM	3435	C	TYR	B	574	66.745	6.452	75.393	1.00	28.82	B
	ATOM	3436	O	TYR	B	574	66.611	5.965	74.264	1.00	28.32	B
	ATOM	3437	N	SER	B	575	67.169	7.692	75.590	1.00	28.07	B
	ATOM	3438	CA	SER	B	575	67.431	8.564	74.461	1.00	27.39	B
40	ATOM	3439	CB	SER	B	575	66.101	9.147	73.980	1.00	27.09	B
	ATOM	3440	OG	SER	B	575	66.260	9.948	72.833	1.00	23.40	B
	ATOM	3441	C	SER	B	575	68.368	9.690	74.832	1.00	27.21	B
	ATOM	3442	O	SER	B	575	68.400	10.124	75.979	1.00	29.42	B
	ATOM	3443	N	THR	B	576	69.131	10.169	73.859	1.00	26.42	B
45	ATOM	3444	CA	THR	B	576	70.036	11.279	74.101	1.00	24.44	B
	ATOM	3445	CB	THR	B	576	71.350	10.794	74.680	1.00	23.42	B
	ATOM	3446	OG1	THR	B	576	72.176	11.925	74.958	1.00	22.28	B
	ATOM	3447	CG2	THR	B	576	72.070	9.898	73.680	1.00	23.95	B
	ATOM	3448	C	THR	B	576	70.314	11.995	72.782	1.00	24.66	B
50	ATOM	3449	O	THR	B	576	70.225	11.405	71.712	1.00	23.66	B
	ATOM	3450	N	ILE	B	577	70.639	13.274	72.843	1.00	25.19	B
	ATOM	3451	CA	ILE	B	577	70.938	13.979	71.615	1.00	24.85	B
	ATOM	3452	CB	ILE	B	577	69.767	14.869	71.172	1.00	23.89	B
	ATOM	3453	CG2	ILE	B	577	70.271	15.939	70.202	1.00	21.80	B

5	ATOM	3454	CG1	ILE	B	577	68.671	14.011	70.538	1.00	23.81	B
	ATOM	3455	CD1	ILE	B	577	67.376	14.750	70.224	1.00	21.31	B
	ATOM	3456	C	ILE	B	577	72.163	14.851	71.802	1.00	26.44	B
	ATOM	3457	O	ILE	B	577	72.324	15.497	72.833	1.00	26.92	B
	ATOM	3458	N	TYR	B	578	73.037	14.850	70.802	1.00	27.45	B
	ATOM	3459	CA	TYR	B	578	74.235	15.672	70.848	1.00	27.93	B
	ATOM	3460	CB	TYR	B	578	75.423	14.925	70.226	1.00	28.17	B
	ATOM	3461	CG	TYR	B	578	76.688	15.757	70.084	1.00	30.25	B
10	ATOM	3462	CD1	TYR	B	578	77.096	16.629	71.089	1.00	28.62	B
	ATOM	3463	CE1	TYR	B	578	78.235	17.416	70.934	1.00	29.38	B
	ATOM	3464	CD2	TYR	B	578	77.464	15.690	68.922	1.00	31.91	B
	ATOM	3465	CE2	TYR	B	578	78.607	16.476	68.762	1.00	30.14	B
15	ATOM	3466	CZ	TYR	B	578	78.980	17.334	69.767	1.00	29.57	B
	ATOM	3467	OH	TYR	B	578	80.082	18.135	69.605	1.00	31.32	B
	ATOM	3468	C	TYR	B	578	73.943	16.980	70.117	1.00	27.87	B
	ATOM	3469	O	TYR	B	578	73.789	17.017	68.897	1.00	27.54	B
	ATOM	3470	N	ASP	B	579	73.832	18.045	70.901	1.00	28.90	B
	ATOM	3471	CA	ASP	B	579	73.551	19.369	70.380	1.00	30.92	B
20	ATOM	3472	CB	ASP	B	579	72.799	20.203	71.416	1.00	30.53	B
	ATOM	3473	CG	ASP	B	579	72.248	21.473	70.839	1.00	34.02	B
	ATOM	3474	OD1	ASP	B	579	72.845	21.995	69.868	1.00	35.60	B
	ATOM	3475	OD2	ASP	B	579	71.219	21.968	71.357	1.00	37.17	B
	ATOM	3476	C	ASP	B	579	74.871	20.026	70.035	1.00	31.94	B
25	ATOM	3477	O	ASP	B	579	75.344	20.923	70.732	1.00	30.49	B
	ATOM	3478	N	HIS	B	580	75.461	19.557	68.945	1.00	34.88	B
	ATOM	3479	CA	HIS	B	580	76.731	20.085	68.492	1.00	38.67	B
	ATOM	3480	CB	HIS	B	580	77.133	19.422	67.170	1.00	40.80	B
	ATOM	3481	CG	HIS	B	580	76.123	19.579	66.080	1.00	44.94	B
	ATOM	3482	CD2	HIS	B	580	76.268	19.900	64.773	1.00	46.55	B
30	ATOM	3483	ND1	HIS	B	580	74.778	19.359	66.276	1.00	47.64	B
	ATOM	3484	CE1	HIS	B	580	74.135	19.532	65.132	1.00	47.95	B
	ATOM	3485	NE2	HIS	B	580	75.016	19.860	64.206	1.00	46.75	B
	ATOM	3486	C	HIS	B	580	76.684	21.601	68.364	1.00	39.17	B
	ATOM	3487	O	HIS	B	580	77.545	22.297	68.907	1.00	40.61	B
35	ATOM	3488	N	GLU	B	581	75.673	22.122	67.681	1.00	39.97	B
	ATOM	3489	CA	GLU	B	581	75.563	23.566	67.529	1.00	40.63	B
	ATOM	3490	CB	GLU	B	581	74.162	23.960	67.078	1.00	42.60	B
	ATOM	3491	CG	GLU	B	581	73.991	25.469	66.960	1.00	46.26	B
40	ATOM	3492	CD	GLU	B	581	72.848	25.853	66.052	1.00	47.68	B
	ATOM	3493	OE1	GLU	B	581	72.857	25.407	64.880	1.00	48.93	B
	ATOM	3494	OE2	GLU	B	581	71.952	26.598	66.508	1.00	48.37	B
	ATOM	3495	C	GLU	B	581	75.871	24.279	68.836	1.00	40.05	B
	ATOM	3496	O	GLU	B	581	76.810	25.063	68.916	1.00	40.37	B
45	ATOM	3497	N	ARG	B	582	75.074	23.998	69.859	1.00	39.74	B
	ATOM	3498	CA	ARG	B	582	75.266	24.622	71.151	1.00	38.74	B
	ATOM	3499	CB	ARG	B	582	73.939	24.647	71.899	1.00	37.10	B
	ATOM	3500	CG	ARG	B	582	73.131	25.905	71.619	1.00	37.06	B
50	ATOM	3501	CD	ARG	B	582	71.654	25.749	71.970	1.00	35.83	B
	ATOM	3502	NE	ARG	B	582	70.962	24.890	71.012	1.00	35.08	B
	ATOM	3503	CZ	ARG	B	582	70.041	25.312	70.154	1.00	34.96	B
	ATOM	3504	NH1	ARG	B	582	69.691	26.591	70.130	1.00	32.75	B
	ATOM	3505	NH2	ARG	B	582	69.466	24.448	69.327	1.00	35.91	B
	ATOM	3506	C	ARG	B	582	76.356	23.971	71.989	1.00	39.71	B
	ATOM	3507	O	ARG	B	582	76.775	24.529	73.003	1.00	40.75	B

	ATOM	3508	N	LYS	B	583	76.825	22.804	71.548	1.00	40.22	B
	ATOM	3509	CA	LYS	B	583	77.881	22.056	72.240	1.00	39.65	B
	ATOM	3510	CB	LYS	B	583	79.089	22.961	72.487	1.00	41.30	B
	ATOM	3511	CG	LYS	B	583	80.401	22.212	72.649	1.00	43.06	B
5	ATOM	3512	CD	LYS	B	583	80.866	21.664	71.311	1.00	46.02	B
	ATOM	3513	CE	LYS	B	583	81.196	22.806	70.367	1.00	46.16	B
	ATOM	3514	NZ	LYS	B	583	82.256	23.657	70.976	1.00	46.38	B
	ATOM	3515	C	LYS	B	583	77.357	21.524	73.574	1.00	38.48	B
	ATOM	3516	O	LYS	B	583	77.990	21.689	74.615	1.00	37.90	B
10	ATOM	3517	N	ARG	B	584	76.202	20.871	73.526	1.00	36.80	B
	ATOM	3518	CA	ARG	B	584	75.575	20.343	74.728	1.00	36.72	B
	ATOM	3519	CB	ARG	B	584	74.436	21.278	75.140	1.00	35.58	B
	ATOM	3520	CG	ARG	B	584	74.930	22.481	75.916	1.00	38.40	B
	ATOM	3521	CD	ARG	B	584	74.542	23.820	75.330	1.00	37.40	B
15	ATOM	3522	NE	ARG	B	584	73.160	24.166	75.635	1.00	39.31	B
	ATOM	3523	CZ	ARG	B	584	72.723	25.408	75.833	1.00	40.87	B
	ATOM	3524	NH1	ARG	B	584	73.556	26.437	75.759	1.00	40.61	B
	ATOM	3525	NH2	ARG	B	584	71.448	25.617	76.122	1.00	40.77	B
	ATOM	3526	C	ARG	B	584	75.045	18.915	74.573	1.00	36.65	B
20	ATOM	3527	O	ARG	B	584	75.211	18.298	73.522	1.00	36.06	B
	ATOM	3528	N	CYS	B	585	74.443	18.372	75.631	1.00	36.04	B
	ATOM	3529	CA	CYS	B	585	73.847	17.043	75.534	1.00	34.78	B
	ATOM	3530	CB	CYS	B	585	74.778	15.936	75.994	1.00	36.01	B
	ATOM	3531	SG	CYS	B	585	73.955	14.322	75.938	1.00	38.57	B
25	ATOM	3532	C	CYS	B	585	72.566	16.929	76.330	1.00	33.64	B
	ATOM	3533	O	CYS	B	585	72.503	17.328	77.495	1.00	33.83	B
	ATOM	3534	N	ILE	B	586	71.544	16.397	75.668	1.00	31.40	B
	ATOM	3535	CA	ILE	B	586	70.247	16.182	76.277	1.00	31.62	B
	ATOM	3536	CB	ILE	B	586	69.079	16.610	75.325	1.00	29.83	B
30	ATOM	3537	CG2	ILE	B	586	67.725	16.305	75.961	1.00	25.17	B
	ATOM	3538	CG1	ILE	B	586	69.155	18.111	75.009	1.00	28.59	B
	ATOM	3539	CD1	ILE	B	586	69.610	18.438	73.588	1.00	27.79	B
	ATOM	3540	C	ILE	B	586	70.135	14.680	76.534	1.00	33.85	B
	ATOM	3541	O	ILE	B	586	70.530	13.882	75.679	1.00	35.25	B
35	ATOM	3542	N	SER	B	587	69.634	14.291	77.712	1.00	34.29	B
	ATOM	3543	CA	SER	B	587	69.428	12.870	78.031	1.00	34.28	B
	ATOM	3544	CB	SER	B	587	70.548	12.320	78.933	1.00	33.74	B
	ATOM	3545	OG	SER	B	587	70.727	13.066	80.122	1.00	34.80	B
	ATOM	3546	C	SER	B	587	68.060	12.648	78.685	1.00	33.99	B
40	ATOM	3547	O	SER	B	587	67.639	13.419	79.546	1.00	32.52	B
	ATOM	3548	N	ALA	B	588	67.355	11.615	78.233	1.00	34.19	B
	ATOM	3549	CA	ALA	B	588	66.054	11.286	78.793	1.00	35.71	B
	ATOM	3550	CB	ALA	B	588	65.006	11.155	77.699	1.00	35.73	B
	ATOM	3551	C	ALA	B	588	66.259	9.960	79.495	1.00	36.25	B
45	ATOM	3552	O	ALA	B	588	66.752	9.016	78.884	1.00	37.28	B
	ATOM	3553	N	SER	B	589	65.929	9.906	80.786	1.00	36.81	B
	ATOM	3554	CA	SER	B	589	66.084	8.684	81.582	1.00	35.90	B
	ATOM	3555	CB	SER	B	589	66.888	8.950	82.851	1.00	34.91	B
	ATOM	3556	OG	SER	B	589	66.512	8.030	83.870	1.00	32.54	B
50	ATOM	3557	C	SER	B	589	64.761	8.093	82.005	1.00	35.49	B
	ATOM	3558	O	SER	B	589	63.714	8.712	81.844	1.00	34.24	B
	ATOM	3559	N	MSE	B	590	64.826	6.883	82.550	1.00	36.42	B
	ATOM	3560	CA	MSE	B	590	63.648	6.188	83.040	1.00	36.64	B
	ATOM	3561	CB	MSE	B	590	63.949	4.702	83.249	1.00	39.18	B

	ATOM	3562	CG	MSE	B	590	62.896	3.948	84.060	1.00	41.10	B
	ATOM	3563	SE	MSE	B	590	63.091	2.012	83.900	1.00	46.30	B
	ATOM	3564	CE	MSE	B	590	61.725	1.645	82.565	1.00	45.20	B
	ATOM	3565	C	MSE	B	590	63.241	6.819	84.361	1.00	35.83	B
5	ATOM	3566	O	MSE	B	590	62.152	6.554	84.860	1.00	35.48	B
	ATOM	3567	N	ASP	B	591	64.116	7.650	84.932	1.00	35.51	B
	ATOM	3568	CA	ASP	B	591	63.791	8.301	86.198	1.00	34.59	B
	ATOM	3569	CB	ASP	B	591	65.051	8.767	86.951	1.00	34.80	B
	ATOM	3570	CG	ASP	B	591	65.874	9.763	86.177	1.00	34.10	B
10	ATOM	3571	OD1	ASP	B	591	65.329	10.459	85.300	1.00	35.66	B
	ATOM	3572	OD2	ASP	B	591	67.081	9.869	86.466	1.00	33.64	B
	ATOM	3573	C	ASP	B	591	62.838	9.463	85.986	1.00	33.76	B
	ATOM	3574	O	ASP	B	591	62.767	10.373	86.801	1.00	31.76	B
	ATOM	3575	N	THR	B	592	62.120	9.418	84.866	1.00	35.29	B
15	ATOM	3576	CA	THR	B	592	61.120	10.419	84.536	1.00	34.85	B
	ATOM	3577	CB	THR	B	592	59.984	10.372	85.631	1.00	34.66	B
	ATOM	3578	OG1	THR	B	592	58.742	10.820	85.079	1.00	38.41	B
	ATOM	3579	CG2	THR	B	592	60.338	11.235	86.830	1.00	34.65	B
	ATOM	3580	C	THR	B	592	61.745	11.811	84.403	1.00	33.52	B
20	ATOM	3581	O	THR	B	592	61.049	12.815	84.455	1.00	33.23	B
	ATOM	3582	N	THR	B	593	63.053	11.858	84.169	1.00	32.55	B
	ATOM	3583	CA	THR	B	593	63.764	13.130	84.070	1.00	32.86	B
	ATOM	3584	CB	THR	B	593	64.786	13.239	85.217	1.00	34.19	B
	ATOM	3585	OG1	THR	B	593	64.082	13.389	86.454	1.00	36.50	B
25	ATOM	3586	CG2	THR	B	593	65.730	14.430	85.018	1.00	38.69	B
	ATOM	3587	C	THR	B	593	64.500	13.423	82.765	1.00	33.21	B
	ATOM	3588	O	THR	B	593	64.856	12.519	82.015	1.00	32.79	B
	ATOM	3589	N	ILE	B	594	64.714	14.705	82.488	1.00	33.30	B
	ATOM	3590	CA	ILE	B	594	65.471	15.103	81.309	1.00	33.34	B
30	ATOM	3591	CB	ILE	B	594	64.612	15.829	80.249	1.00	31.46	B
	ATOM	3592	CG2	ILE	B	594	65.496	16.322	79.132	1.00	29.37	B
	ATOM	3593	CG1	ILE	B	594	63.534	14.902	79.690	1.00	32.39	B
	ATOM	3594	CD1	ILE	B	594	62.436	15.642	78.920	1.00	27.89	B
	ATOM	3595	C	ILE	B	594	66.497	16.104	81.824	1.00	35.21	B
35	ATOM	3596	O	ILE	B	594	66.161	16.973	82.628	1.00	37.01	B
	ATOM	3597	N	ARG	B	595	67.749	15.977	81.402	1.00	35.67	B
	ATOM	3598	CA	ARG	B	595	68.735	16.947	81.834	1.00	36.60	B
	ATOM	3599	CB	ARG	B	595	69.447	16.482	83.104	1.00	39.57	B
	ATOM	3600	CG	ARG	B	595	70.237	15.219	83.020	1.00	41.84	B
40	ATOM	3601	CD	ARG	B	595	70.672	14.865	84.428	1.00	43.91	B
	ATOM	3602	NE	ARG	B	595	69.554	14.397	85.240	1.00	44.22	B
	ATOM	3603	CZ	ARG	B	595	69.658	14.054	86.518	1.00	45.26	B
	ATOM	3604	NH1	ARG	B	595	70.848	14.147	87.121	1.00	44.50	B
	ATOM	3605	NH2	ARG	B	595	68.586	13.589	87.170	1.00	41.38	B
45	ATOM	3606	C	ARG	B	595	69.731	17.324	80.751	1.00	36.11	B
	ATOM	3607	O	ARG	B	595	70.067	16.512	79.880	1.00	36.08	B
	ATOM	3608	N	ILE	B	596	70.173	18.579	80.791	1.00	34.47	B
	ATOM	3609	CA	ILE	B	596	71.116	19.084	79.807	1.00	34.38	B
	ATOM	3610	CB	ILE	B	596	70.662	20.479	79.263	1.00	35.15	B
50	ATOM	3611	CG2	ILE	B	596	71.746	21.058	78.357	1.00	35.63	B
	ATOM	3612	CG1	ILE	B	596	69.390	20.334	78.401	1.00	36.12	B
	ATOM	3613	CD1	ILE	B	596	68.175	19.723	79.073	1.00	29.57	B
	ATOM	3614	C	ILE	B	596	72.515	19.174	80.415	1.00	32.98	B
	ATOM	3615	O	ILE	B	596	72.679	19.563	81.570	1.00	30.78	B

	ATOM	3616	N	TRP	B	597	73.520	18.795	79.638	1.00	33.10	B
	ATOM	3617	CA	TRP	B	597	74.892	18.821	80.124	1.00	34.71	B
	ATOM	3618	CB	TRP	B	597	75.493	17.404	80.117	1.00	34.39	B
	ATOM	3619	CG	TRP	B	597	74.577	16.341	80.645	1.00	33.10	B
5	ATOM	3620	CD2	TRP	B	597	74.691	15.653	81.893	1.00	33.20	B
	ATOM	3621	CE2	TRP	B	597	73.607	14.752	81.974	1.00	33.38	B
	ATOM	3622	CE3	TRP	B	597	75.599	15.713	82.956	1.00	33.08	B
	ATOM	3623	CD1	TRP	B	597	73.463	15.842	80.035	1.00	33.47	B
	ATOM	3624	NE1	TRP	B	597	72.874	14.884	80.826	1.00	32.94	B
10	ATOM	3625	CZ2	TRP	B	597	73.411	13.912	83.072	1.00	33.63	B
	ATOM	3626	CZ3	TRP	B	597	75.406	14.878	84.051	1.00	32.87	B
	ATOM	3627	CH2	TRP	B	597	74.314	13.989	84.101	1.00	33.13	B
	ATOM	3628	C	TRP	B	597	75.725	19.726	79.229	1.00	35.90	B
	ATOM	3629	O	TRP	B	597	75.455	19.837	78.028	1.00	36.19	B
15	ATOM	3630	N	ASP	B	598	76.731	20.372	79.817	1.00	36.61	B
	ATOM	3631	CA	ASP	B	598	77.631	21.265	79.082	1.00	38.19	B
	ATOM	3632	CB	ASP	B	598	78.156	22.369	80.018	1.00	36.98	B
	ATOM	3633	CG	ASP	B	598	78.999	23.410	79.291	1.00	37.20	B
	ATOM	3634	OD1	ASP	B	598	79.604	23.089	78.240	1.00	36.53	B
20	ATOM	3635	OD2	ASP	B	598	79.059	24.553	79.786	1.00	37.52	B
	ATOM	3636	C	ASP	B	598	78.806	20.426	78.574	1.00	39.00	B
	ATOM	3637	O	ASP	B	598	79.670	20.050	79.349	1.00	39.73	B
	ATOM	3638	N	LEU	B	599	78.847	20.126	77.282	1.00	40.71	B
	ATOM	3639	CA	LEU	B	599	79.942	19.320	76.747	1.00	42.08	B
25	ATOM	3640	CB	LEU	B	599	79.593	18.805	75.344	1.00	40.52	B
	ATOM	3641	CG	LEU	B	599	78.606	17.628	75.251	1.00	40.62	B
	ATOM	3642	CD1	LEU	B	599	79.264	16.437	74.600	1.00	38.01	B
	ATOM	3643	CD2	LEU	B	599	78.096	17.258	76.638	1.00	38.10	B
	ATOM	3644	C	LEU	B	599	81.295	20.025	76.721	1.00	43.84	B
30	ATOM	3645	O	LEU	B	599	82.256	19.494	76.165	1.00	44.70	B
	ATOM	3646	N	GLU	B	600	81.373	21.216	77.315	1.00	44.72	B
	ATOM	3647	CA	GLU	B	600	82.637	21.941	77.358	1.00	45.68	B
	ATOM	3648	CB	GLU	B	600	82.412	23.413	77.697	1.00	48.89	B
	ATOM	3649	CG	GLU	B	600	83.460	24.367	77.128	1.00	52.63	B
35	ATOM	3650	CD	GLU	B	600	84.762	24.375	77.924	1.00	56.18	B
	ATOM	3651	OE1	GLU	B	600	84.739	24.763	79.120	1.00	58.19	B
	ATOM	3652	OE2	GLU	B	600	85.811	23.997	77.353	1.00	57.88	B
	ATOM	3653	C	GLU	B	600	83.480	21.254	78.419	1.00	45.43	B
	ATOM	3654	O	GLU	B	600	84.683	21.083	78.242	1.00	46.22	B
40	ATOM	3655	N	ASN	B	605	82.844	20.855	79.518	1.00	44.31	B
	ATOM	3656	CA	ASN	B	605	83.543	20.124	80.568	1.00	43.89	B
	ATOM	3657	CB	ASN	B	605	84.285	21.077	81.520	1.00	46.09	B
	ATOM	3658	CG	ASN	B	605	85.808	21.121	81.248	1.00	50.14	B
	ATOM	3659	OD1	ASN	B	605	86.508	20.093	81.348	1.00	50.14	B
45	ATOM	3660	ND2	ASN	B	605	86.320	22.314	80.900	1.00	49.96	B
	ATOM	3661	C	ASN	B	605	82.630	19.186	81.346	1.00	41.67	B
	ATOM	3662	O	ASN	B	605	82.756	19.054	82.554	1.00	43.82	B
	ATOM	3663	N	GLY	B	606	81.718	18.525	80.638	1.00	38.96	B
	ATOM	3664	CA	GLY	B	606	80.804	17.584	81.268	1.00	35.37	B
50	ATOM	3665	C	GLY	B	606	80.059	18.044	82.512	1.00	34.56	B
	ATOM	3666	O	GLY	B	606	79.668	17.231	83.350	1.00	32.65	B
	ATOM	3667	N	GLU	B	607	79.846	19.348	82.622	1.00	34.50	B
	ATOM	3668	CA	GLU	B	607	79.147	19.921	83.757	1.00	35.96	B
	ATOM	3669	CB	GLU	B	607	79.616	21.367	83.976	1.00	36.06	B

	ATOM	3670	CG	GLU	B	607	81.114	21.618	83.763	1.00	39.20	B
	ATOM	3671	CD	GLU	B	607	81.468	21.981	82.321	1.00	39.57	B
	ATOM	3672	OE1	GLU	B	607	80.924	21.353	81.405	1.00	41.63	B
	ATOM	3673	OE2	GLU	B	607	82.301	22.877	82.097	1.00	38.72	B
5	ATOM	3674	C	GLU	B	607	77.622	19.892	83.504	1.00	37.13	B
	ATOM	3675	O	GLU	B	607	77.157	20.165	82.391	1.00	36.86	B
	ATOM	3676	N	LEU	B	608	76.850	19.539	84.530	1.00	37.44	B
	ATOM	3677	CA	LEU	B	608	75.395	19.513	84.412	1.00	37.50	B
	ATOM	3678	CB	LEU	B	608	74.753	18.822	85.622	1.00	37.08	B
10	ATOM	3679	CG	LEU	B	608	73.218	18.925	85.723	1.00	37.03	B
	ATOM	3680	CD1	LEU	B	608	72.593	18.036	84.658	1.00	36.12	B
	ATOM	3681	CD2	LEU	B	608	72.724	18.533	87.127	1.00	34.40	B
	ATOM	3682	C	LEU	B	608	74.912	20.962	84.339	1.00	38.65	B
	ATOM	3683	O	LEU	B	608	75.442	21.833	85.030	1.00	38.26	B
15	ATOM	3684	N	MSE	B	625	73.902	21.210	83.510	1.00	39.30	B
	ATOM	3685	CA	MSE	B	625	73.368	22.553	83.329	1.00	39.07	B
	ATOM	3686	CB	MSE	B	625	73.266	22.890	81.842	1.00	41.00	B
	ATOM	3687	CG	MSE	B	625	74.571	23.323	81.217	1.00	43.67	B
	ATOM	3688	SE	MSE	B	625	74.423	23.805	79.359	1.00	50.89	B
20	ATOM	3689	CE	MSE	B	625	73.882	25.650	79.578	1.00	45.39	B
	ATOM	3690	C	MSE	B	625	72.008	22.737	83.946	1.00	38.75	B
	ATOM	3691	O	MSE	B	625	71.803	23.605	84.795	1.00	39.63	B
	ATOM	3692	N	TYR	B	626	71.068	21.919	83.495	1.00	38.88	B
	ATOM	3693	CA	TYR	B	626	69.700	22.003	83.975	1.00	37.07	B
25	ATOM	3694	CB	TYR	B	626	68.861	22.841	83.016	1.00	35.69	B
	ATOM	3695	CG	TYR	B	626	69.457	24.160	82.618	1.00	34.35	B
	ATOM	3696	CD1	TYR	B	626	69.560	25.199	83.535	1.00	33.06	B
	ATOM	3697	CE1	TYR	B	626	70.013	26.447	83.150	1.00	32.14	B
	ATOM	3698	CD2	TYR	B	626	69.840	24.397	81.295	1.00	34.51	B
30	ATOM	3699	CE2	TYR	B	626	70.296	25.646	80.896	1.00	33.07	B
	ATOM	3700	CZ	TYR	B	626	70.373	26.671	81.833	1.00	31.79	B
	ATOM	3701	OH	TYR	B	626	70.753	27.933	81.446	1.00	28.57	B
	ATOM	3702	C	TYR	B	626	69.067	20.635	84.040	1.00	36.34	B
	ATOM	3703	O	TYR	B	626	69.528	19.690	83.410	1.00	37.33	B
35	ATOM	3704	N	THR	B	627	67.992	20.560	84.809	1.00	36.28	B
	ATOM	3705	CA	THR	B	627	67.203	19.357	84.958	1.00	34.33	B
	ATOM	3706	CB	THR	B	627	67.340	18.744	86.373	1.00	32.94	B
	ATOM	3707	OG1	THR	B	627	68.684	18.292	86.562	1.00	30.38	B
	ATOM	3708	CG2	THR	B	627	66.391	17.544	86.535	1.00	32.04	B
40	ATOM	3709	C	THR	B	627	65.764	19.808	84.719	1.00	34.24	B
	ATOM	3710	O	THR	B	627	65.248	20.700	85.400	1.00	33.46	B
	ATOM	3711	N	LEU	B	628	65.137	19.204	83.722	1.00	34.53	B
	ATOM	3712	CA	LEU	B	628	63.772	19.525	83.355	1.00	34.30	B
	ATOM	3713	CB	LEU	B	628	63.636	19.558	81.835	1.00	35.54	B
45	ATOM	3714	CG	LEU	B	628	64.814	20.120	81.056	1.00	36.04	B
	ATOM	3715	CD1	LEU	B	628	64.459	20.071	79.591	1.00	37.79	B
	ATOM	3716	CD2	LEU	B	628	65.137	21.538	81.500	1.00	35.35	B
	ATOM	3717	C	LEU	B	628	62.844	18.454	83.886	1.00	32.68	B
	ATOM	3718	O	LEU	B	628	63.055	17.261	83.647	1.00	33.72	B
50	ATOM	3719	N	GLN	B	629	61.805	18.882	84.582	1.00	30.62	B
	ATOM	3720	CA	GLN	B	629	60.849	17.949	85.127	1.00	30.70	B
	ATOM	3721	CB	GLN	B	629	60.774	18.082	86.647	1.00	28.58	B
	ATOM	3722	CG	GLN	B	629	59.867	17.050	87.257	1.00	27.57	B
	ATOM	3723	CD	GLN	B	629	60.402	15.655	87.063	1.00	28.68	B

	ATOM	3724	OE1	GLN	B	629	59.733	14.775	86.486	1.00	28.51	B
	ATOM	3725	NE2	GLN	B	629	61.620	15.434	87.545	1.00	27.17	B
	ATOM	3726	C	GLN	B	629	59.473	18.204	84.544	1.00	31.36	B
	ATOM	3727	O	GLN	B	629	58.677	18.958	85.104	1.00	31.90	B
5	ATOM	3728	N	GLY	B	630	59.183	17.567	83.424	1.00	31.87	B
	ATOM	3729	CA	GLY	B	630	57.889	17.767	82.804	1.00	33.15	B
	ATOM	3730	C	GLY	B	630	57.254	16.467	82.364	1.00	33.55	B
	ATOM	3731	O	GLY	B	630	56.511	16.425	81.385	1.00	35.60	B
	ATOM	3732	N	HIS	B	631	57.553	15.400	83.092	1.00	32.53	B
10	ATOM	3733	CA	HIS	B	631	57.023	14.083	82.784	1.00	30.78	B
	ATOM	3734	CB	HIS	B	631	57.943	13.368	81.792	1.00	28.27	B
	ATOM	3735	CG	HIS	B	631	58.054	14.052	80.466	1.00	24.31	B
	ATOM	3736	CD2	HIS	B	631	59.003	14.874	79.965	1.00	21.91	B
	ATOM	3737	ND1	HIS	B	631	57.118	13.895	79.467	1.00	26.41	B
15	ATOM	3738	CE1	HIS	B	631	57.487	14.587	78.405	1.00	22.90	B
	ATOM	3739	NE2	HIS	B	631	58.629	15.190	78.681	1.00	22.42	B
	ATOM	3740	C	HIS	B	631	56.957	13.302	84.091	1.00	30.77	B
	ATOM	3741	O	HIS	B	631	57.834	13.437	84.948	1.00	30.31	B
	ATOM	3742	N	THR	B	632	55.916	12.489	84.239	1.00	31.40	B
20	ATOM	3743	CA	THR	B	632	55.716	11.690	85.447	1.00	32.08	B
	ATOM	3744	CB	THR	B	632	54.281	11.742	85.914	1.00	32.58	B
	ATOM	3745	OG1	THR	B	632	53.446	11.255	84.860	1.00	33.44	B
	ATOM	3746	CG2	THR	B	632	53.877	13.151	86.274	1.00	31.80	B
	ATOM	3747	C	THR	B	632	55.990	10.233	85.152	1.00	32.55	B
25	ATOM	3748	O	THR	B	632	55.790	9.367	86.000	1.00	33.19	B
	ATOM	3749	N	ALA	B	633	56.442	9.963	83.941	1.00	32.22	B
	ATOM	3750	CA	ALA	B	633	56.721	8.604	83.537	1.00	32.78	B
	ATOM	3751	CB	ALA	B	633	55.596	8.106	82.627	1.00	33.46	B
	ATOM	3752	C	ALA	B	633	58.048	8.649	82.786	1.00	33.18	B
30	ATOM	3753	O	ALA	B	633	58.570	9.730	82.526	1.00	34.34	B
	ATOM	3754	N	LEU	B	634	58.606	7.502	82.419	1.00	32.23	B
	ATOM	3755	CA	LEU	B	634	59.881	7.559	81.718	1.00	31.56	B
	ATOM	3756	CB	LEU	B	634	60.531	6.176	81.610	1.00	32.84	B
	ATOM	3757	CG	LEU	B	634	59.855	5.099	80.783	1.00	33.81	B
35	ATOM	3758	CD1	LEU	B	634	58.372	5.151	81.095	1.00	37.82	B
	ATOM	3759	CD2	LEU	B	634	60.122	5.300	79.304	1.00	32.77	B
	ATOM	3760	C	LEU	B	634	59.787	8.214	80.353	1.00	29.60	B
	ATOM	3761	O	LEU	B	634	58.807	8.072	79.620	1.00	27.99	B
	ATOM	3762	N	VAL	B	635	60.835	8.961	80.045	1.00	27.96	B
40	ATOM	3763	CA	VAL	B	635	60.945	9.688	78.803	1.00	25.69	B
	ATOM	3764	CB	VAL	B	635	61.584	11.046	79.038	1.00	27.20	B
	ATOM	3765	CG1	VAL	B	635	61.377	11.926	77.810	1.00	28.07	B
	ATOM	3766	CG2	VAL	B	635	61.000	11.679	80.302	1.00	25.75	B
	ATOM	3767	C	VAL	B	635	61.827	8.948	77.840	1.00	23.61	B
45	ATOM	3768	O	VAL	B	635	63.046	9.033	77.942	1.00	23.52	B
	ATOM	3769	N	GLY	B	636	61.219	8.248	76.891	1.00	22.88	B
	ATOM	3770	CA	GLY	B	636	61.998	7.488	75.928	1.00	22.35	B
	ATOM	3771	C	GLY	B	636	62.224	8.089	74.550	1.00	23.37	B
	ATOM	3772	O	GLY	B	636	62.907	7.480	73.736	1.00	24.09	B
50	ATOM	3773	N	LEU	B	637	61.656	9.262	74.277	1.00	23.96	B
	ATOM	3774	CA	LEU	B	637	61.827	9.904	72.981	1.00	23.22	B
	ATOM	3775	CB	LEU	B	637	60.503	9.934	72.228	1.00	22.08	B
	ATOM	3776	CG	LEU	B	637	59.913	8.534	72.102	1.00	21.07	B
	ATOM	3777	CD1	LEU	B	637	58.494	8.554	71.516	1.00	18.52	B

	ATOM	3778	CD2	LEU	B	637	60.863	7.724	71.261	1.00	18.91	B
	ATOM	3779	C	LEU	B	637	62.328	11.317	73.164	1.00	25.24	B
	ATOM	3780	O	LEU	B	637	62.058	11.945	74.197	1.00	25.36	B
	ATOM	3781	N	LEU	B	638	63.048	11.797	72.142	1.00	26.06	B
5	ATOM	3782	CA	LEU	B	638	63.635	13.147	72.077	1.00	25.52	B
	ATOM	3783	CB	LEU	B	638	64.907	13.258	72.926	1.00	25.76	B
	ATOM	3784	CG	LEU	B	638	64.857	13.321	74.453	1.00	26.07	B
	ATOM	3785	CD1	LEU	B	638	66.285	13.384	74.983	1.00	27.82	B
	ATOM	3786	CD2	LEU	B	638	64.073	14.535	74.897	1.00	25.88	B
10	ATOM	3787	C	LEU	B	638	64.022	13.494	70.653	1.00	25.17	B
	ATOM	3788	O	LEU	B	638	64.529	12.644	69.919	1.00	25.44	B
	ATOM	3789	N	ARG	B	639	63.771	14.744	70.268	1.00	25.50	B
	ATOM	3790	CA	ARG	B	639	64.126	15.260	68.942	1.00	25.66	B
	ATOM	3791	CB	ARG	B	639	63.033	14.936	67.901	1.00	25.21	B
15	ATOM	3792	CG	ARG	B	639	62.720	13.427	67.878	1.00	28.60	B
	ATOM	3793	CD	ARG	B	639	62.173	12.811	66.583	1.00	28.49	B
	ATOM	3794	NE	ARG	B	639	63.252	12.293	65.730	1.00	30.47	B
	ATOM	3795	CZ	ARG	B	639	63.131	11.295	64.851	1.00	30.02	B
	ATOM	3796	NH1	ARG	B	639	61.970	10.668	64.684	1.00	27.71	B
20	ATOM	3797	NH2	ARG	B	639	64.183	10.926	64.123	1.00	32.50	B
	ATOM	3798	C	ARG	B	639	64.379	16.760	69.078	1.00	25.33	B
	ATOM	3799	O	ARG	B	639	63.738	17.442	69.877	1.00	24.41	B
	ATOM	3800	N	LEU	B	640	65.355	17.258	68.332	1.00	26.36	B
	ATOM	3801	CA	LEU	B	640	65.707	18.661	68.408	1.00	27.00	B
25	ATOM	3802	CB	LEU	B	640	67.214	18.808	68.563	1.00	28.00	B
	ATOM	3803	CG	LEU	B	640	67.688	19.504	69.834	1.00	27.72	B
	ATOM	3804	CD1	LEU	B	640	69.188	19.757	69.737	1.00	25.31	B
	ATOM	3805	CD2	LEU	B	640	66.914	20.802	70.019	1.00	25.63	B
	ATOM	3806	C	LEU	B	640	65.263	19.432	67.189	1.00	27.04	B
30	ATOM	3807	O	LEU	B	640	65.759	19.210	66.097	1.00	27.98	B
	ATOM	3808	N	SER	B	641	64.310	20.329	67.373	1.00	29.24	B
	ATOM	3809	CA	SER	B	641	63.828	21.138	66.271	1.00	30.57	B
	ATOM	3810	CB	SER	B	641	62.359	21.509	66.504	1.00	31.54	B
	ATOM	3811	OG	SER	B	641	62.025	22.763	65.944	1.00	30.17	B
35	ATOM	3812	C	SER	B	641	64.718	22.366	66.277	1.00	31.05	B
	ATOM	3813	O	SER	B	641	65.499	22.560	67.198	1.00	32.13	B
	ATOM	3814	N	ASP	B	642	64.628	23.194	65.254	1.00	32.29	B
	ATOM	3815	CA	ASP	B	642	65.472	24.373	65.210	1.00	32.45	B
	ATOM	3816	CB	ASP	B	642	65.293	25.059	63.870	1.00	36.58	B
40	ATOM	3817	CG	ASP	B	642	66.575	25.652	63.360	1.00	40.19	B
	ATOM	3818	OD1	ASP	B	642	67.336	24.914	62.681	1.00	41.18	B
	ATOM	3819	OD2	ASP	B	642	66.816	26.848	63.661	1.00	42.03	B
	ATOM	3820	C	ASP	B	642	65.140	25.348	66.344	1.00	31.30	B
	ATOM	3821	O	ASP	B	642	65.996	26.095	66.809	1.00	28.33	B
45	ATOM	3822	N	LYS	B	643	63.876	25.332	66.759	1.00	30.65	B
	ATOM	3823	CA	LYS	B	643	63.373	26.190	67.818	1.00	28.54	B
	ATOM	3824	CB	LYS	B	643	62.069	26.888	67.407	1.00	28.11	B
	ATOM	3825	CG	LYS	B	643	62.141	27.807	66.210	1.00	30.60	B
	ATOM	3826	CD	LYS	B	643	63.196	28.902	66.364	1.00	32.54	B
50	ATOM	3827	CE	LYS	B	643	63.332	29.736	65.070	1.00	33.58	B
	ATOM	3828	NZ	LYS	B	643	63.760	28.917	63.873	1.00	33.86	B
	ATOM	3829	C	LYS	B	643	63.047	25.391	69.077	1.00	28.15	B
	ATOM	3830	O	LYS	B	643	63.019	25.951	70.163	1.00	28.92	B
	ATOM	3831	N	PHE	B	644	62.787	24.094	68.957	1.00	26.09	B

	ATOM	3832	CA	PHE	B	644	62.413	23.353	70.152	1.00	24.49	B
	ATOM	3833	CB	PHE	B	644	60.931	22.958	70.115	1.00	21.46	B
	ATOM	3834	CG	PHE	B	644	60.015	24.023	69.613	1.00	20.17	B
	ATOM	3835	CD1	PHE	B	644	59.720	24.125	68.258	1.00	22.46	B
5	ATOM	3836	CD2	PHE	B	644	59.404	24.896	70.493	1.00	20.58	B
	ATOM	3837	CE1	PHE	B	644	58.816	25.079	67.783	1.00	20.21	B
	ATOM	3838	CE2	PHE	B	644	58.501	25.855	70.035	1.00	20.45	B
	ATOM	3839	CZ	PHE	B	644	58.207	25.942	68.674	1.00	20.84	B
	ATOM	3840	C	PHE	B	644	63.186	22.087	70.457	1.00	25.20	B
10	ATOM	3841	O	PHE	B	644	63.886	21.534	69.613	1.00	24.80	B
	ATOM	3842	N	LEU	B	645	63.054	21.649	71.701	1.00	25.69	B
	ATOM	3843	CA	LEU	B	645	63.630	20.396	72.151	1.00	25.88	B
	ATOM	3844	CB	LEU	B	645	64.547	20.586	73.359	1.00	26.05	B
	ATOM	3845	CG	LEU	B	645	64.777	19.327	74.233	1.00	27.77	B
15	ATOM	3846	CD1	LEU	B	645	66.044	18.602	73.852	1.00	28.34	B
	ATOM	3847	CD2	LEU	B	645	64.864	19.739	75.692	1.00	29.93	B
	ATOM	3848	C	LEU	B	645	62.349	19.704	72.590	1.00	26.32	B
	ATOM	3849	O	LEU	B	645	61.743	20.096	73.591	1.00	27.97	B
	ATOM	3850	N	VAL	B	646	61.910	18.706	71.834	1.00	25.54	B
20	ATOM	3851	CA	VAL	B	646	60.688	18.005	72.191	1.00	25.91	B
	ATOM	3852	CB	VAL	B	646	59.892	17.651	70.918	1.00	25.69	B
	ATOM	3853	CG1	VAL	B	646	58.554	17.036	71.293	1.00	26.37	B
	ATOM	3854	CG2	VAL	B	646	59.681	18.909	70.069	1.00	23.92	B
	ATOM	3855	C	VAL	B	646	61.003	16.734	72.986	1.00	26.60	B
25	ATOM	3856	O	VAL	B	646	62.051	16.130	72.780	1.00	27.76	B
	ATOM	3857	N	SER	B	647	60.121	16.358	73.916	1.00	27.17	B
	ATOM	3858	CA	SER	B	647	60.281	15.130	74.711	1.00	27.29	B
	ATOM	3859	CB	SER	B	647	60.956	15.417	76.054	1.00	27.08	B
	ATOM	3860	OG	SER	B	647	60.210	16.325	76.850	1.00	27.93	B
30	ATOM	3861	C	SER	B	647	58.905	14.512	74.942	1.00	28.49	B
	ATOM	3862	O	SER	B	647	57.943	15.227	75.219	1.00	29.23	B
	ATOM	3863	N	ALA	B	648	58.819	13.189	74.800	1.00	28.67	B
	ATOM	3864	CA	ALA	B	648	57.568	12.454	74.976	1.00	28.62	B
	ATOM	3865	CB	ALA	B	648	57.093	11.906	73.630	1.00	28.17	B
35	ATOM	3866	C	ALA	B	648	57.760	11.306	75.972	1.00	30.51	B
	ATOM	3867	O	ALA	B	648	58.756	10.577	75.898	1.00	31.42	B
	ATOM	3868	N	ALA	B	649	56.807	11.146	76.894	1.00	30.32	B
	ATOM	3869	CA	ALA	B	649	56.883	10.098	77.911	1.00	30.33	B
	ATOM	3870	CB	ALA	B	649	56.720	10.700	79.305	1.00	29.35	B
40	ATOM	3871	C	ALA	B	649	55.863	8.988	77.711	1.00	31.09	B
	ATOM	3872	O	ALA	B	649	54.995	9.080	76.850	1.00	30.54	B
	ATOM	3873	N	ALA	B	650	55.981	7.941	78.530	1.00	32.95	B
	ATOM	3874	CA	ALA	B	650	55.103	6.768	78.483	1.00	32.69	B
	ATOM	3875	CB	ALA	B	650	55.783	5.597	79.194	1.00	30.66	B
45	ATOM	3876	C	ALA	B	650	53.733	7.019	79.098	1.00	33.02	B
	ATOM	3877	O	ALA	B	650	52.941	6.091	79.251	1.00	32.69	B
	ATOM	3878	N	ASP	B	651	53.471	8.270	79.463	1.00	34.34	B
	ATOM	3879	CA	ASP	B	651	52.200	8.661	80.063	1.00	35.15	B
	ATOM	3880	CB	ASP	B	651	52.456	9.528	81.287	1.00	36.84	B
50	ATOM	3881	CG	ASP	B	651	53.402	10.663	80.993	1.00	40.07	B
	ATOM	3882	OD1	ASP	B	651	53.652	10.935	79.800	1.00	40.99	B
	ATOM	3883	OD2	ASP	B	651	53.895	11.299	81.950	1.00	43.26	B
	ATOM	3884	C	ASP	B	651	51.347	9.441	79.068	1.00	35.49	B
	ATOM	3885	O	ASP	B	651	50.282	9.948	79.418	1.00	35.89	B

	ATOM	3886	N	GLY	B	652	51.833	9.542	77.834	1.00	34.99	B
	ATOM	3887	CA	GLY	B	652	51.110	10.260	76.802	1.00	34.08	B
	ATOM	3888	C	GLY	B	652	51.434	11.738	76.730	1.00	34.36	B
	ATOM	3889	O	GLY	B	652	50.877	12.449	75.891	1.00	36.08	B
5	ATOM	3890	N	SER	B	653	52.336	12.198	77.595	1.00	32.03	B
	ATOM	3891	CA	SER	B	653	52.720	13.605	77.635	1.00	30.49	B
	ATOM	3892	CB	SER	B	653	53.176	13.995	79.050	1.00	31.53	B
	ATOM	3893	OG	SER	B	653	54.387	13.358	79.428	1.00	31.63	B
	ATOM	3894	C	SER	B	653	53.810	13.962	76.633	1.00	29.75	B
10	ATOM	3895	O	SER	B	653	54.702	13.165	76.361	1.00	28.99	B
	ATOM	3896	N	ILE	B	654	53.733	15.175	76.097	1.00	30.15	B
	ATOM	3897	CA	ILE	B	654	54.703	15.655	75.115	1.00	30.00	B
	ATOM	3898	CB	ILE	B	654	54.083	15.708	73.706	1.00	29.09	B
	ATOM	3899	CG2	ILE	B	654	55.115	16.144	72.686	1.00	28.47	B
15	ATOM	3900	CG1	ILE	B	654	53.548	14.336	73.318	1.00	28.15	B
	ATOM	3901	CD1	ILE	B	654	52.204	14.400	72.675	1.00	30.38	B
	ATOM	3902	C	ILE	B	654	55.109	17.061	75.508	1.00	30.87	B
	ATOM	3903	O	ILE	B	654	54.285	17.974	75.484	1.00	32.52	B
	ATOM	3904	N	ARG	B	655	56.371	17.241	75.878	1.00	30.22	B
20	ATOM	3905	CA	ARG	B	655	56.835	18.570	76.271	1.00	29.48	B
	ATOM	3906	CB	ARG	B	655	57.614	18.492	77.589	1.00	31.26	B
	ATOM	3907	CG	ARG	B	655	56.773	18.219	78.827	1.00	34.00	B
	ATOM	3908	CD	ARG	B	655	56.140	19.500	79.287	1.00	40.70	B
	ATOM	3909	NE	ARG	B	655	55.601	19.484	80.657	1.00	45.23	B
25	ATOM	3910	CZ	ARG	B	655	54.582	18.735	81.075	1.00	48.41	B
	ATOM	3911	NH1	ARG	B	655	53.979	17.909	80.234	1.00	49.81	B
	ATOM	3912	NH2	ARG	B	655	54.137	18.847	82.324	1.00	50.20	B
	ATOM	3913	C	ARG	B	655	57.712	19.195	75.187	1.00	28.14	B
	ATOM	3914	O	ARG	B	655	58.462	18.501	74.500	1.00	27.90	B
30	ATOM	3915	N	GLY	B	656	57.582	20.507	75.033	1.00	26.00	B
	ATOM	3916	CA	GLY	B	656	58.365	21.237	74.065	1.00	24.28	B
	ATOM	3917	C	GLY	B	656	59.047	22.348	74.830	1.00	24.73	B
	ATOM	3918	O	GLY	B	656	58.384	23.228	75.386	1.00	26.11	B
	ATOM	3919	N	TRP	B	657	60.373	22.296	74.883	1.00	24.11	B
35	ATOM	3920	CA	TRP	B	657	61.163	23.294	75.601	1.00	23.50	B
	ATOM	3921	CB	TRP	B	657	62.139	22.602	76.550	1.00	22.75	B
	ATOM	3922	CG	TRP	B	657	61.579	21.381	77.189	1.00	21.95	B
	ATOM	3923	CD2	TRP	B	657	61.213	21.230	78.562	1.00	19.79	B
	ATOM	3924	CE2	TRP	B	657	60.639	19.948	78.698	1.00	20.88	B
40	ATOM	3925	CE3	TRP	B	657	61.320	22.048	79.691	1.00	19.86	B
	ATOM	3926	CD1	TRP	B	657	61.231	20.213	76.566	1.00	20.79	B
	ATOM	3927	NE1	TRP	B	657	60.657	19.350	77.469	1.00	20.21	B
	ATOM	3928	CZ2	TRP	B	657	60.160	19.478	79.926	1.00	21.49	B
	ATOM	3929	CZ3	TRP	B	657	60.846	21.570	80.915	1.00	20.44	B
45	ATOM	3930	CH2	TRP	B	657	60.278	20.301	81.019	1.00	20.36	B
	ATOM	3931	C	TRP	B	657	61.966	24.122	74.610	1.00	24.96	B
	ATOM	3932	O	TRP	B	657	62.262	23.673	73.498	1.00	24.34	B
	ATOM	3933	N	ASP	B	658	62.331	25.331	75.014	1.00	26.03	B
	ATOM	3934	CA	ASP	B	658	63.126	26.181	74.137	1.00	28.03	B
50	ATOM	3935	CB	ASP	B	658	63.307	27.565	74.741	1.00	28.12	B
	ATOM	3936	CG	ASP	B	658	64.031	28.494	73.805	1.00	29.75	B
	ATOM	3937	OD1	ASP	B	658	65.264	28.356	73.641	1.00	28.58	B
	ATOM	3938	OD2	ASP	B	658	63.352	29.351	73.209	1.00	31.24	B
	ATOM	3939	C	ASP	B	658	64.498	25.538	73.961	1.00	28.55	B

	ATOM	3940	O	ASP	B	658	65.168	25.253	74.948	1.00	31.11	B
	ATOM	3941	N	ALA	B	659	64.924	25.334	72.719	1.00	27.30	B
	ATOM	3942	CA	ALA	B	659	66.209	24.689	72.443	1.00	28.28	B
	ATOM	3943	CB	ALA	B	659	66.413	24.549	70.945	1.00	26.59	B
5	ATOM	3944	C	ALA	B	659	67.430	25.362	73.047	1.00	29.08	B
	ATOM	3945	O	ALA	B	659	68.518	24.784	73.067	1.00	30.37	B
	ATOM	3946	N	ASN	B	660	67.272	26.577	73.544	1.00	29.04	B
	ATOM	3947	CA	ASN	B	660	68.419	27.256	74.090	1.00	29.15	B
	ATOM	3948	CB	ASN	B	660	68.618	28.573	73.361	1.00	32.02	B
10	ATOM	3949	CG	ASN	B	660	69.953	29.185	73.646	1.00	36.15	B
	ATOM	3950	OD1	ASN	B	660	70.999	28.600	73.342	1.00	39.04	B
	ATOM	3951	ND2	ASN	B	660	69.939	30.371	74.238	1.00	38.31	B
	ATOM	3952	C	ASN	B	660	68.334	27.474	75.582	1.00	28.96	B
	ATOM	3953	O	ASN	B	660	69.262	27.138	76.301	1.00	30.76	B
15	ATOM	3954	N	ASP	B	661	67.225	28.024	76.059	1.00	28.20	B
	ATOM	3955	CA	ASP	B	661	67.073	28.249	77.485	1.00	26.87	B
	ATOM	3956	CB	ASP	B	661	66.553	29.663	77.745	1.00	29.19	B
	ATOM	3957	CG	ASP	B	661	65.311	29.984	76.942	1.00	30.92	B
	ATOM	3958	OD1	ASP	B	661	65.314	31.019	76.232	1.00	32.39	B
20	ATOM	3959	OD2	ASP	B	661	64.334	29.209	77.023	1.00	30.85	B
	ATOM	3960	C	ASP	B	661	66.147	27.217	78.129	1.00	26.15	B
	ATOM	3961	O	ASP	B	661	66.041	27.165	79.346	1.00	28.27	B
	ATOM	3962	N	TYR	B	662	65.474	26.409	77.317	1.00	22.94	B
	ATOM	3963	CA	TYR	B	662	64.590	25.365	77.819	1.00	21.57	B
25	ATOM	3964	CB	TYR	B	662	65.407	24.340	78.623	1.00	20.55	B
	ATOM	3965	CG	TYR	B	662	66.647	23.879	77.871	1.00	21.52	B
	ATOM	3966	CD1	TYR	B	662	67.867	24.533	78.019	1.00	19.76	B
	ATOM	3967	CE1	TYR	B	662	68.960	24.193	77.231	1.00	18.58	B
	ATOM	3968	CD2	TYR	B	662	66.567	22.861	76.919	1.00	20.80	B
30	ATOM	3969	CE2	TYR	B	662	67.659	22.519	76.126	1.00	18.36	B
	ATOM	3970	CZ	TYR	B	662	68.851	23.192	76.287	1.00	18.65	B
	ATOM	3971	OH	TYR	B	662	69.935	22.893	75.493	1.00	18.77	B
	ATOM	3972	C	TYR	B	662	63.346	25.808	78.604	1.00	21.16	B
	ATOM	3973	O	TYR	B	662	62.835	25.068	79.443	1.00	20.62	B
35	ATOM	3974	N	SER	B	663	62.864	27.015	78.327	1.00	21.52	B
	ATOM	3975	CA	SER	B	663	61.642	27.500	78.954	1.00	21.24	B
	ATOM	3976	CB	SER	B	663	61.458	28.993	78.699	1.00	19.14	B
	ATOM	3977	OG	SER	B	663	61.441	29.273	77.312	1.00	19.19	B
	ATOM	3978	C	SER	B	663	60.496	26.728	78.294	1.00	21.60	B
40	ATOM	3979	O	SER	B	663	60.585	26.352	77.123	1.00	20.87	B
	ATOM	3980	N	ARG	B	664	59.436	26.489	79.057	1.00	22.75	B
	ATOM	3981	CA	ARG	B	664	58.267	25.755	78.592	1.00	23.75	B
	ATOM	3982	CB	ARG	B	664	57.317	25.544	79.764	1.00	26.18	B
	ATOM	3983	CG	ARG	B	664	58.032	24.928	80.948	1.00	33.56	B
45	ATOM	3984	CD	ARG	B	664	57.130	24.061	81.812	1.00	39.29	B
	ATOM	3985	NE	ARG	B	664	57.925	23.331	82.801	1.00	43.83	B
	ATOM	3986	CZ	ARG	B	664	57.446	22.404	83.625	1.00	47.40	B
	ATOM	3987	NH1	ARG	B	664	56.158	22.076	83.594	1.00	48.81	B
	ATOM	3988	NH2	ARG	B	664	58.265	21.796	84.474	1.00	48.40	B
50	ATOM	3989	C	ARG	B	664	57.540	26.436	77.433	1.00	23.79	B
	ATOM	3990	O	ARG	B	664	56.829	27.420	77.632	1.00	23.72	B
	ATOM	3991	N	LYS	B	665	57.702	25.886	76.228	1.00	23.87	B
	ATOM	3992	CA	LYS	B	665	57.091	26.453	75.021	1.00	24.18	B
	ATOM	3993	CB	LYS	B	665	58.099	26.400	73.869	1.00	25.26	B

5	ATOM	3994	CG	LYS	B	665	59.088	27.551	73.869	1.00	26.13	B
	ATOM	3995	CD	LYS	B	665	58.423	28.779	73.292	1.00	31.91	B
	ATOM	3996	CE	LYS	B	665	59.389	29.964	73.126	1.00	34.51	B
	ATOM	3997	NZ	LYS	B	665	59.804	30.608	74.426	1.00	40.98	B
	ATOM	3998	C	LYS	B	665	55.760	25.844	74.588	1.00	22.25	B
10	ATOM	3999	O	LYS	B	665	54.943	26.514	73.956	1.00	21.84	B
	ATOM	4000	N	PHE	B	666	55.555	24.574	74.917	1.00	22.07	B
	ATOM	4001	CA	PHE	B	666	54.308	23.875	74.604	1.00	22.00	B
	ATOM	4002	CB	PHE	B	666	54.109	23.776	73.076	1.00	21.53	B
	ATOM	4003	CG	PHE	B	666	55.017	22.786	72.373	1.00	21.45	B
15	ATOM	4004	CD1	PHE	B	666	54.744	21.420	72.408	1.00	21.12	B
	ATOM	4005	CD2	PHE	B	666	56.134	23.218	71.664	1.00	20.63	B
	ATOM	4006	CE1	PHE	B	666	55.562	20.506	71.758	1.00	17.08	B
	ATOM	4007	CE2	PHE	B	666	56.951	22.303	71.015	1.00	19.89	B
	ATOM	4008	CZ	PHE	B	666	56.659	20.947	71.066	1.00	17.19	B
20	ATOM	4009	C	PHE	B	666	54.272	22.494	75.288	1.00	22.61	B
	ATOM	4010	O	PHE	B	666	55.323	21.938	75.618	1.00	24.01	B
	ATOM	4011	N	SER	B	667	53.068	21.973	75.538	1.00	22.74	B
	ATOM	4012	CA	SER	B	667	52.891	20.674	76.200	1.00	23.29	B
	ATOM	4013	CB	SER	B	667	52.827	20.831	77.717	1.00	22.23	B
25	ATOM	4014	OG	SER	B	667	51.487	20.937	78.145	1.00	23.02	B
	ATOM	4015	C	SER	B	667	51.596	20.014	75.737	1.00	24.06	B
	ATOM	4016	O	SER	B	667	50.525	20.635	75.772	1.00	23.18	B
	ATOM	4017	N	TYR	B	668	51.703	18.751	75.321	1.00	24.19	B
	ATOM	4018	CA	TYR	B	668	50.554	17.999	74.834	1.00	24.45	B
30	ATOM	4019	CB	TYR	B	668	50.633	17.810	73.324	1.00	24.25	B
	ATOM	4020	CG	TYR	B	668	50.638	19.089	72.543	1.00	24.38	B
	ATOM	4021	CD1	TYR	B	668	51.752	19.452	71.785	1.00	23.71	B
	ATOM	4022	CE1	TYR	B	668	51.759	20.610	71.024	1.00	24.24	B
	ATOM	4023	CD2	TYR	B	668	49.519	19.924	72.528	1.00	24.84	B
35	ATOM	4024	CE2	TYR	B	668	49.514	21.091	71.770	1.00	25.84	B
	ATOM	4025	CZ	TYR	B	668	50.643	21.426	71.017	1.00	26.29	B
	ATOM	4026	OH	TYR	B	668	50.656	22.572	70.263	1.00	27.29	B
	ATOM	4027	C	TYR	B	668	50.391	16.634	75.462	1.00	23.76	B
	ATOM	4028	O	TYR	B	668	51.364	15.944	75.751	1.00	23.84	B
40	ATOM	4029	N	HIS	B	669	49.144	16.223	75.612	1.00	24.21	B
	ATOM	4030	CA	HIS	B	669	48.864	14.948	76.225	1.00	26.26	B
	ATOM	4031	CB	HIS	B	669	48.329	15.214	77.623	1.00	27.79	B
	ATOM	4032	CG	HIS	B	669	48.682	14.159	78.607	1.00	30.20	B
	ATOM	4033	CD2	HIS	B	669	48.174	12.921	78.797	1.00	32.47	B
45	ATOM	4034	ND1	HIS	B	669	49.695	14.309	79.526	1.00	30.16	B
	ATOM	4035	CE1	HIS	B	669	49.796	13.205	80.244	1.00	31.69	B
	ATOM	4036	NE2	HIS	B	669	48.884	12.347	79.822	1.00	32.65	B
	ATOM	4037	C	HIS	B	669	47.836	14.157	75.421	1.00	25.01	B
	ATOM	4038	O	HIS	B	669	46.743	14.662	75.167	1.00	25.41	B
50	ATOM	4039	N	HIS	B	670	48.163	12.936	75.003	1.00	24.99	B
	ATOM	4040	CA	HIS	B	670	47.173	12.152	74.262	1.00	26.67	B
	ATOM	4041	CB	HIS	B	670	47.788	10.894	73.644	1.00	26.67	B
	ATOM	4042	CG	HIS	B	670	48.526	11.149	72.367	1.00	28.25	B
	ATOM	4043	CD2	HIS	B	670	49.149	12.266	71.911	1.00	27.02	B
50	ATOM	4044	ND1	HIS	B	670	48.704	10.187	71.399	1.00	28.10	B
	ATOM	4045	CE1	HIS	B	670	49.404	10.697	70.398	1.00	27.39	B
	ATOM	4046	NE2	HIS	B	670	49.685	11.955	70.687	1.00	25.82	B
	ATOM	4047	C	HIS	B	670	46.033	11.766	75.198	1.00	28.34	B

	ATOM	4048	O	HIS	B	670	46.255	11.292	76.320	1.00	28.98	B
	ATOM	4049	N	THR	B	671	44.812	11.970	74.717	1.00	29.18	B
	ATOM	4050	CA	THR	B	671	43.597	11.706	75.479	1.00	29.09	B
	ATOM	4051	CB	THR	B	671	42.363	11.963	74.600	1.00	28.97	B
5	ATOM	4052	OG1	THR	B	671	42.582	11.400	73.299	1.00	29.48	B
	ATOM	4053	CG2	THR	B	671	42.108	13.457	74.470	1.00	28.78	B
	ATOM	4054	C	THR	B	671	43.434	10.341	76.127	1.00	27.51	B
	ATOM	4055	O	THR	B	671	42.911	10.245	77.234	1.00	26.92	B
	ATOM	4056	N	ASN	B	672	43.857	9.291	75.436	1.00	28.14	B
10	ATOM	4057	CA	ASN	B	672	43.715	7.936	75.961	1.00	29.14	B
	ATOM	4058	CB	ASN	B	672	43.528	6.943	74.808	1.00	30.07	B
	ATOM	4059	CG	ASN	B	672	44.774	6.802	73.954	1.00	31.70	B
	ATOM	4060	OD1	ASN	B	672	45.721	7.592	74.082	1.00	32.55	B
	ATOM	4061	ND2	ASN	B	672	44.779	5.803	73.067	1.00	30.68	B
15	ATOM	4062	C	ASN	B	672	44.911	7.538	76.819	1.00	27.80	B
	ATOM	4063	O	ASN	B	672	45.184	6.354	77.040	1.00	25.74	B
	ATOM	4064	N	LEU	B	673	45.624	8.554	77.283	1.00	27.49	B
	ATOM	4065	CA	LEU	B	673	46.771	8.370	78.152	1.00	28.57	B
	ATOM	4066	CB	LEU	B	673	46.267	8.132	79.581	1.00	26.43	B
20	ATOM	4067	CG	LEU	B	673	45.295	9.183	80.132	1.00	27.88	B
	ATOM	4068	CD1	LEU	B	673	44.949	8.826	81.572	1.00	28.51	B
	ATOM	4069	CD2	LEU	B	673	45.898	10.581	80.067	1.00	26.47	B
	ATOM	4070	C	LEU	B	673	47.711	7.243	77.727	1.00	28.78	B
	ATOM	4071	O	LEU	B	673	48.353	6.613	78.560	1.00	28.06	B
25	ATOM	4072	N	SER	B	674	47.805	6.992	76.431	1.00	29.36	B
	ATOM	4073	CA	SER	B	674	48.676	5.926	75.960	1.00	29.70	B
	ATOM	4074	CB	SER	B	674	48.207	5.459	74.585	1.00	32.41	B
	ATOM	4075	OG	SER	B	674	46.859	5.039	74.652	1.00	35.35	B
	ATOM	4076	C	SER	B	674	50.140	6.353	75.892	1.00	27.54	B
30	ATOM	4077	O	SER	B	674	50.438	7.522	75.678	1.00	27.24	B
	ATOM	4078	N	ALA	B	675	51.053	5.407	76.074	1.00	25.24	B
	ATOM	4079	CA	ALA	B	675	52.455	5.748	76.006	1.00	24.53	B
	ATOM	4080	CB	ALA	B	675	53.304	4.573	76.393	1.00	25.14	B
	ATOM	4081	C	ALA	B	675	52.793	6.179	74.589	1.00	25.51	B
35	ATOM	4082	O	ALA	B	675	52.484	5.472	73.610	1.00	26.90	B
	ATOM	4083	N	ILE	B	676	53.429	7.340	74.485	1.00	23.80	B
	ATOM	4084	CA	ILE	B	676	53.824	7.880	73.200	1.00	23.18	B
	ATOM	4085	CB	ILE	B	676	54.457	9.276	73.354	1.00	22.28	B
	ATOM	4086	CG2	ILE	B	676	54.960	9.749	71.999	1.00	26.37	B
40	ATOM	4087	CG1	ILE	B	676	53.437	10.265	73.913	1.00	20.36	B
	ATOM	4088	CD1	ILE	B	676	52.158	10.388	73.112	1.00	19.30	B
	ATOM	4089	C	ILE	B	676	54.835	6.966	72.505	1.00	23.03	B
	ATOM	4090	O	ILE	B	676	55.939	6.770	73.005	1.00	22.66	B
	ATOM	4091	N	THR	B	677	54.454	6.432	71.344	1.00	23.91	B
45	ATOM	4092	CA	THR	B	677	55.310	5.536	70.554	1.00	24.45	B
	ATOM	4093	CB	THR	B	677	54.495	4.625	69.663	1.00	21.85	B
	ATOM	4094	OG1	THR	B	677	53.512	3.966	70.447	1.00	21.96	B
	ATOM	4095	CG2	THR	B	677	55.406	3.590	69.020	1.00	27.86	B
	ATOM	4096	C	THR	B	677	56.291	6.286	69.642	1.00	26.36	B
50	ATOM	4097	O	THR	B	677	57.469	5.953	69.580	1.00	26.98	B
	ATOM	4098	N	THR	B	678	55.787	7.252	68.884	1.00	27.47	B
	ATOM	4099	CA	THR	B	678	56.647	8.070	68.046	1.00	28.85	B
	ATOM	4100	CB	THR	B	678	56.939	7.483	66.615	1.00	31.08	B
	ATOM	4101	OG1	THR	B	678	55.731	7.007	66.003	1.00	33.29	B

5	ATOM	4102	CG2	THR	B	678	57.971	6.378	66.698	1.00	35.12	B
	ATOM	4103	C	THR	B	678	56.070	9.447	67.831	1.00	28.29	B
	ATOM	4104	O	THR	B	678	54.934	9.742	68.215	1.00	29.19	B
	ATOM	4105	N	PHE	B	679	56.889	10.273	67.194	1.00	27.12	B
	ATOM	4106	CA	PHE	B	679	56.552	11.621	66.835	1.00	24.71	B
10	ATOM	4107	CB	PHE	B	679	56.246	12.453	68.085	1.00	25.37	B
	ATOM	4108	CG	PHE	B	679	57.481	12.945	68.829	1.00	24.77	B
	ATOM	4109	CD1	PHE	B	679	58.206	14.061	68.374	1.00	21.98	B
	ATOM	4110	CD2	PHE	B	679	57.916	12.293	69.990	1.00	24.36	B
	ATOM	4111	CE1	PHE	B	679	59.331	14.509	69.063	1.00	19.92	B
15	ATOM	4112	CE2	PHE	B	679	59.032	12.736	70.671	1.00	22.18	B
	ATOM	4113	CZ	PHE	B	679	59.739	13.845	70.207	1.00	21.94	B
	ATOM	4114	C	PHE	B	679	57.762	12.174	66.095	1.00	24.89	B
	ATOM	4115	O	PHE	B	679	58.894	11.669	66.212	1.00	21.91	B
	ATOM	4116	N	TYR	B	680	57.504	13.231	65.338	1.00	25.98	B
20	ATOM	4117	CA	TYR	B	680	58.516	13.918	64.557	1.00	25.00	B
	ATOM	4118	CB	TYR	B	680	58.418	13.438	63.104	1.00	23.81	B
	ATOM	4119	CG	TYR	B	680	59.668	13.711	62.317	1.00	27.68	B
	ATOM	4120	CD1	TYR	B	680	60.795	12.881	62.429	1.00	26.50	B
	ATOM	4121	CE1	TYR	B	680	62.003	13.232	61.812	1.00	27.92	B
25	ATOM	4122	CD2	TYR	B	680	59.780	14.881	61.559	1.00	28.23	B
	ATOM	4123	CE2	TYR	B	680	60.971	15.237	60.949	1.00	27.91	B
	ATOM	4124	CZ	TYR	B	680	62.074	14.427	61.080	1.00	28.40	B
	ATOM	4125	OH	TYR	B	680	63.253	14.870	60.531	1.00	31.86	B
	ATOM	4126	C	TYR	B	680	58.122	15.405	64.735	1.00	23.73	B
30	ATOM	4127	O	TYR	B	680	56.975	15.684	65.090	1.00	22.88	B
	ATOM	4128	N	VAL	B	681	59.053	16.340	64.520	1.00	23.01	B
	ATOM	4129	CA	VAL	B	681	58.785	17.781	64.698	1.00	21.87	B
	ATOM	4130	CB	VAL	B	681	59.211	18.315	66.071	1.00	20.14	B
	ATOM	4131	CG1	VAL	B	681	58.030	18.505	66.979	1.00	18.83	B
35	ATOM	4132	CG2	VAL	B	681	60.254	17.397	66.641	1.00	21.44	B
	ATOM	4133	C	VAL	B	681	59.556	18.695	63.781	1.00	21.58	B
	ATOM	4134	O	VAL	B	681	60.694	18.427	63.399	1.00	19.29	B
	ATOM	4135	N	SER	B	682	58.928	19.818	63.480	1.00	21.27	B
	ATOM	4136	CA	SER	B	682	59.554	20.864	62.685	1.00	20.48	B
40	ATOM	4137	CB	SER	B	682	58.923	20.956	61.300	1.00	19.96	B
	ATOM	4138	OG	SER	B	682	57.535	21.230	61.396	1.00	20.38	B
	ATOM	4139	C	SER	B	682	59.174	22.065	63.518	1.00	20.44	B
	ATOM	4140	O	SER	B	682	58.332	21.944	64.407	1.00	22.67	B
	ATOM	4141	N	ASP	B	683	59.797	23.207	63.275	1.00	19.98	B
45	ATOM	4142	CA	ASP	B	683	59.441	24.394	64.036	1.00	19.73	B
	ATOM	4143	CB	ASP	B	683	60.212	25.638	63.547	1.00	20.26	B
	ATOM	4144	CG	ASP	B	683	61.708	25.650	63.959	1.00	21.54	B
	ATOM	4145	OD1	ASP	B	683	62.132	24.891	64.860	1.00	19.41	B
	ATOM	4146	OD2	ASP	B	683	62.468	26.460	63.377	1.00	22.23	B
50	ATOM	4147	C	ASP	B	683	57.936	24.665	63.889	1.00	18.98	B
	ATOM	4148	O	ASP	B	683	57.351	25.254	64.782	1.00	19.03	B
	ATOM	4149	N	ASN	B	684	57.311	24.214	62.800	1.00	18.67	B
	ATOM	4150	CA	ASN	B	684	55.888	24.482	62.579	1.00	20.77	B
	ATOM	4151	CB	ASN	B	684	55.644	24.891	61.136	1.00	20.60	B
	ATOM	4152	CG	ASN	B	684	56.303	26.196	60.780	1.00	23.83	B
	ATOM	4153	OD1	ASN	B	684	56.062	27.233	61.419	1.00	24.57	B
	ATOM	4154	ND2	ASN	B	684	57.134	26.165	59.741	1.00	23.71	B
	ATOM	4155	C	ASN	B	684	54.874	23.392	62.886	1.00	22.90	B

	ATOM	4156	O	ASN	B	684	53.687	23.690	63.077	1.00	22.24	B
	ATOM	4157	N	ILE	B	685	55.327	22.140	62.890	1.00	23.24	B
	ATOM	4158	CA	ILE	B	685	54.449	20.997	63.118	1.00	20.82	B
	ATOM	4159	CB	ILE	B	685	54.156	20.257	61.778	1.00	19.24	B
5	ATOM	4160	CG2	ILE	B	685	53.256	19.057	62.014	1.00	18.99	B
	ATOM	4161	CG1	ILE	B	685	53.488	21.211	60.784	1.00	17.58	B
	ATOM	4162	CD1	ILE	B	685	52.067	21.562	61.120	1.00	17.99	B
	ATOM	4163	C	ILE	B	685	55.037	19.993	64.100	1.00	21.40	B
	ATOM	4164	O	ILE	B	685	56.263	19.961	64.315	1.00	21.31	B
10	ATOM	4165	N	LEU	B	686	54.137	19.207	64.697	1.00	20.50	B
	ATOM	4166	CA	LEU	B	686	54.461	18.147	65.648	1.00	21.98	B
	ATOM	4167	CB	LEU	B	686	54.273	18.612	67.108	1.00	23.37	B
	ATOM	4168	CG	LEU	B	686	54.138	17.518	68.189	1.00	24.30	B
	ATOM	4169	CD1	LEU	B	686	55.479	16.866	68.430	1.00	24.15	B
15	ATOM	4170	CD2	LEU	B	686	53.595	18.098	69.475	1.00	22.84	B
	ATOM	4171	C	LEU	B	686	53.475	17.026	65.361	1.00	22.92	B
	ATOM	4172	O	LEU	B	686	52.297	17.167	65.650	1.00	25.29	B
	ATOM	4173	N	VAL	B	687	53.927	15.924	64.780	1.00	21.99	B
	ATOM	4174	CA	VAL	B	687	53.018	14.817	64.511	1.00	21.64	B
20	ATOM	4175	CB	VAL	B	687	53.186	14.346	63.000	1.00	22.41	B
	ATOM	4176	CG1	VAL	B	687	52.604	12.949	62.796	1.00	21.78	B
	ATOM	4177	CG2	VAL	B	687	52.476	15.325	62.052	1.00	19.88	B
	ATOM	4178	C	VAL	B	687	53.345	13.700	65.542	1.00	21.43	B
	ATOM	4179	O	VAL	B	687	54.476	13.202	65.599	1.00	21.65	B
25	ATOM	4180	N	SER	B	688	52.387	13.330	66.390	1.00	21.20	B
	ATOM	4181	CA	SER	B	688	52.654	12.302	67.412	1.00	21.07	B
	ATOM	4182	CB	SER	B	688	52.601	12.920	68.812	1.00	21.19	B
	ATOM	4183	OG	SER	B	688	51.336	13.509	69.074	1.00	19.67	B
	ATOM	4184	C	SER	B	688	51.706	11.118	67.373	1.00	21.57	B
30	ATOM	4185	O	SER	B	688	50.511	11.265	67.104	1.00	21.58	B
	ATOM	4186	N	GLY	B	689	52.221	9.935	67.674	1.00	23.31	B
	ATOM	4187	CA	GLY	B	689	51.348	8.778	67.635	1.00	25.20	B
	ATOM	4188	C	GLY	B	689	51.498	7.793	68.779	1.00	26.22	B
	ATOM	4189	O	GLY	B	689	52.590	7.549	69.295	1.00	26.74	B
35	ATOM	4190	N	SER	B	690	50.372	7.245	69.200	1.00	26.47	B
	ATOM	4191	CA	SER	B	690	50.350	6.247	70.253	1.00	29.04	B
	ATOM	4192	CB	SER	B	690	49.977	6.881	71.601	1.00	30.51	B
	ATOM	4193	OG	SER	B	690	48.577	7.150	71.674	1.00	31.85	B
	ATOM	4194	C	SER	B	690	49.261	5.262	69.818	1.00	29.64	B
40	ATOM	4195	O	SER	B	690	48.624	5.462	68.788	1.00	31.71	B
	ATOM	4196	N	GLU	B	691	49.037	4.213	70.599	1.00	29.52	B
	ATOM	4197	CA	GLU	B	691	48.005	3.239	70.280	1.00	28.36	B
	ATOM	4198	CB	GLU	B	691	47.857	2.282	71.452	1.00	28.07	B
	ATOM	4199	CG	GLU	B	691	46.563	1.512	71.496	1.00	32.75	B
45	ATOM	4200	CD	GLU	B	691	46.531	0.499	72.635	1.00	35.90	B
	ATOM	4201	OE1	GLU	B	691	47.285	-0.507	72.575	1.00	37.07	B
	ATOM	4202	OE2	GLU	B	691	45.751	0.712	73.594	1.00	36.72	B
	ATOM	4203	C	GLU	B	691	46.689	3.970	70.013	1.00	27.98	B
	ATOM	4204	O	GLU	B	691	46.356	4.921	70.713	1.00	29.12	B
50	ATOM	4205	N	ASN	B	692	45.968	3.554	68.974	1.00	27.34	B
	ATOM	4206	CA	ASN	B	692	44.678	4.159	68.617	1.00	27.55	B
	ATOM	4207	CB	ASN	B	692	43.625	3.832	69.671	1.00	30.51	B
	ATOM	4208	CG	ASN	B	692	43.363	2.347	69.797	1.00	33.53	B
	ATOM	4209	OD1	ASN	B	692	42.997	1.866	70.874	1.00	34.93	B

	ATOM	4210	ND2	ASN	B	692	43.537	1.607	68.694	1.00	36.41	B
	ATOM	4211	C	ASN	B	692	44.671	5.671	68.417	1.00	28.06	B
	ATOM	4212	O	ASN	B	692	43.611	6.271	68.227	1.00	27.85	B
	ATOM	4213	N	GLN	B	693	45.836	6.300	68.455	1.00	27.40	B
5	ATOM	4214	CA	GLN	B	693	45.883	7.737	68.270	1.00	26.47	B
	ATOM	4215	CB	GLN	B	693	46.046	8.410	69.627	1.00	26.45	B
	ATOM	4216	CG	GLN	B	693	44.860	8.235	70.547	1.00	27.10	B
	ATOM	4217	CD	GLN	B	693	44.499	9.523	71.245	1.00	27.21	B
	ATOM	4218	OE1	GLN	B	693	45.360	10.211	71.776	1.00	28.92	B
10	ATOM	4219	NE2	GLN	B	693	43.224	9.859	71.243	1.00	29.30	B
	ATOM	4220	C	GLN	B	693	46.999	8.200	67.320	1.00	26.29	B
	ATOM	4221	O	GLN	B	693	48.105	7.655	67.332	1.00	27.55	B
	ATOM	4222	N	PHE	B	694	46.700	9.196	66.487	1.00	24.60	B
	ATOM	4223	CA	PHE	B	694	47.675	9.771	65.551	1.00	22.51	B
15	ATOM	4224	CB	PHE	B	694	47.612	9.073	64.184	1.00	20.48	B
	ATOM	4225	CG	PHE	B	694	48.701	9.499	63.210	1.00	20.42	B
	ATOM	4226	CD1	PHE	B	694	49.967	8.922	63.241	1.00	20.85	B
	ATOM	4227	CD2	PHE	B	694	48.441	10.465	62.237	1.00	21.71	B
	ATOM	4228	CE1	PHE	B	694	50.956	9.301	62.312	1.00	21.35	B
20	ATOM	4229	CE2	PHE	B	694	49.421	10.851	61.304	1.00	20.94	B
	ATOM	4230	CZ	PHE	B	694	50.674	10.269	61.343	1.00	20.97	B
	ATOM	4231	C	PHE	B	694	47.234	11.227	65.445	1.00	22.04	B
	ATOM	4232	O	PHE	B	694	46.146	11.508	64.951	1.00	22.64	B
	ATOM	4233	N	ASN	B	695	48.065	12.142	65.947	1.00	22.40	B
25	ATOM	4234	CA	ASN	B	695	47.741	13.570	65.946	1.00	22.71	B
	ATOM	4235	CB	ASN	B	695	47.542	14.102	67.383	1.00	24.16	B
	ATOM	4236	CG	ASN	B	695	46.687	13.194	68.246	1.00	27.03	B
	ATOM	4237	OD1	ASN	B	695	47.145	12.735	69.297	1.00	30.17	B
	ATOM	4238	ND2	ASN	B	695	45.441	12.930	67.817	1.00	28.07	B
30	ATOM	4239	C	ASN	B	695	48.762	14.477	65.261	1.00	21.75	B
	ATOM	4240	O	ASN	B	695	49.960	14.194	65.232	1.00	20.80	B
	ATOM	4241	N	ILE	B	696	48.248	15.588	64.734	1.00	21.52	B
	ATOM	4242	CA	ILE	B	696	49.024	16.622	64.045	1.00	20.16	B
	ATOM	4243	CB	ILE	B	696	48.592	16.711	62.556	1.00	17.92	B
35	ATOM	4244	CG2	ILE	B	696	49.367	17.768	61.821	1.00	16.21	B
	ATOM	4245	CG1	ILE	B	696	48.860	15.371	61.883	1.00	16.96	B
	ATOM	4246	CD1	ILE	B	696	48.335	15.277	60.471	1.00	14.78	B
	ATOM	4247	C	ILE	B	696	48.732	17.922	64.803	1.00	20.71	B
	ATOM	4248	O	ILE	B	696	47.589	18.207	65.167	1.00	20.57	B
40	ATOM	4249	N	TYR	B	697	49.779	18.690	65.057	1.00	21.04	B
	ATOM	4250	CA	TYR	B	697	49.651	19.916	65.816	1.00	22.01	B
	ATOM	4251	CB	TYR	B	697	50.334	19.746	67.174	1.00	22.18	B
	ATOM	4252	CG	TYR	B	697	49.748	18.654	68.027	1.00	22.67	B
	ATOM	4253	CD1	TYR	B	697	48.702	18.919	68.917	1.00	21.46	B
45	ATOM	4254	CE1	TYR	B	697	48.167	17.910	69.717	1.00	20.34	B
	ATOM	4255	CD2	TYR	B	697	50.244	17.349	67.952	1.00	22.41	B
	ATOM	4256	CE2	TYR	B	697	49.717	16.331	68.746	1.00	22.87	B
	ATOM	4257	CZ	TYR	B	697	48.685	16.615	69.627	1.00	21.85	B
	ATOM	4258	OH	TYR	B	697	48.212	15.607	70.431	1.00	22.33	B
50	ATOM	4259	C	TYR	B	697	50.244	21.121	65.112	1.00	23.61	B
	ATOM	4260	O	TYR	B	697	51.334	21.080	64.538	1.00	25.65	B
	ATOM	4261	N	ASN	B	698	49.491	22.202	65.162	1.00	23.81	B
	ATOM	4262	CA	ASN	B	698	49.913	23.449	64.594	1.00	23.42	B
	ATOM	4263	CB	ASN	B	698	48.680	24.254	64.224	1.00	26.51	B

	ATOM	4264	CG	ASN	B	698	49.020	25.531	63.512	1.00	28.61	B
	ATOM	4265	OD1	ASN	B	698	49.959	26.238	63.897	1.00	28.06	B
	ATOM	4266	ND2	ASN	B	698	48.255	25.849	62.472	1.00	29.88	B
	ATOM	4267	C	ASN	B	698	50.658	24.079	65.778	1.00	23.71	B
5	ATOM	4268	O	ASN	B	698	50.047	24.586	66.726	1.00	22.24	B
	ATOM	4269	N	LEU	B	699	51.980	23.982	65.732	1.00	23.60	B
	ATOM	4270	CA	LEU	B	699	52.841	24.497	66.773	1.00	24.06	B
	ATOM	4271	CB	LEU	B	699	54.270	24.037	66.517	1.00	22.91	B
	ATOM	4272	CG	LEU	B	699	54.837	22.996	67.475	1.00	23.91	B
10	ATOM	4273	CD1	LEU	B	699	53.784	21.972	67.874	1.00	24.32	B
	ATOM	4274	CD2	LEU	B	699	56.028	22.362	66.832	1.00	22.79	B
	ATOM	4275	C	LEU	B	699	52.801	26.001	66.862	1.00	25.53	B
	ATOM	4276	O	LEU	B	699	53.498	26.580	67.681	1.00	27.08	B
	ATOM	4277	N	ARG	B	700	52.004	26.631	66.002	1.00	26.51	B
15	ATOM	4278	CA	ARG	B	700	51.863	28.087	65.997	1.00	25.40	B
	ATOM	4279	CB	ARG	B	700	51.489	28.600	64.609	1.00	27.54	B
	ATOM	4280	CG	ARG	B	700	52.549	28.502	63.543	1.00	28.72	B
	ATOM	4281	CD	ARG	B	700	53.706	29.422	63.820	1.00	31.33	B
	ATOM	4282	NE	ARG	B	700	54.598	29.480	62.671	1.00	34.27	B
20	ATOM	4283	CZ	ARG	B	700	54.233	29.908	61.464	1.00	36.22	B
	ATOM	4284	NH1	ARG	B	700	52.989	30.318	61.259	1.00	35.49	B
	ATOM	4285	NH2	ARG	B	700	55.107	29.920	60.457	1.00	38.36	B
	ATOM	4286	C	ARG	B	700	50.724	28.431	66.942	1.00	24.24	B
	ATOM	4287	O	ARG	B	700	50.914	29.118	67.928	1.00	22.77	B
25	ATOM	4288	N	SER	B	701	49.532	27.949	66.620	1.00	23.91	B
	ATOM	4289	CA	SER	B	701	48.358	28.202	67.435	1.00	23.69	B
	ATOM	4290	CB	SER	B	701	47.105	27.928	66.633	1.00	21.95	B
	ATOM	4291	OG	SER	B	701	47.096	26.574	66.220	1.00	21.41	B
	ATOM	4292	C	SER	B	701	48.342	27.281	68.627	1.00	25.56	B
30	ATOM	4293	O	SER	B	701	47.546	27.467	69.541	1.00	27.95	B
	ATOM	4294	N	GLY	B	702	49.207	26.273	68.606	1.00	25.80	B
	ATOM	4295	CA	GLY	B	702	49.252	25.311	69.688	1.00	25.16	B
	ATOM	4296	C	GLY	B	702	48.080	24.351	69.601	1.00	25.57	B
	ATOM	4297	O	GLY	B	702	47.963	23.464	70.427	1.00	27.20	B
35	ATOM	4298	N	LYS	B	703	47.221	24.498	68.597	1.00	26.86	B
	ATOM	4299	CA	LYS	B	703	46.049	23.630	68.485	1.00	29.85	B
	ATOM	4300	CB	LYS	B	703	44.846	24.452	67.982	1.00	31.50	B
	ATOM	4301	CG	LYS	B	703	44.521	25.679	68.857	1.00	35.32	B
	ATOM	4302	CD	LYS	B	703	43.066	26.160	68.704	1.00	35.78	B
40	ATOM	4303	CE	LYS	B	703	42.529	26.768	70.007	1.00	39.24	B
	ATOM	4304	NZ	LYS	B	703	42.643	25.841	71.218	1.00	39.02	B
	ATOM	4305	C	LYS	B	703	46.199	22.357	67.631	1.00	29.87	B
	ATOM	4306	O	LYS	B	703	47.079	22.245	66.786	1.00	31.67	B
	ATOM	4307	N	LEU	B	704	45.314	21.403	67.868	1.00	29.38	B
45	ATOM	4308	CA	LEU	B	704	45.319	20.152	67.149	1.00	29.31	B
	ATOM	4309	CB	LEU	B	704	44.445	19.169	67.892	1.00	28.56	B
	ATOM	4310	CG	LEU	B	704	44.409	17.731	67.419	1.00	29.17	B
	ATOM	4311	CD1	LEU	B	704	45.768	17.030	67.620	1.00	29.83	B
	ATOM	4312	CD2	LEU	B	704	43.340	17.041	68.206	1.00	28.68	B
50	ATOM	4313	C	LEU	B	704	44.732	20.390	65.772	1.00	30.18	B
	ATOM	4314	O	LEU	B	704	43.610	20.880	65.669	1.00	32.27	B
	ATOM	4315	N	VAL	B	705	45.458	20.053	64.709	1.00	30.79	B
	ATOM	4316	CA	VAL	B	705	44.908	20.275	63.371	1.00	31.43	B
	ATOM	4317	CB	VAL	B	705	46.012	20.551	62.322	1.00	30.01	B

	ATOM	4318	CG1	VAL	B	705	45.368	20.883	60.976	1.00	28.32	B
	ATOM	4319	CG2	VAL	B	705	46.889	21.685	62.776	1.00	29.54	B
	ATOM	4320	C	VAL	B	705	44.069	19.087	62.904	1.00	32.61	B
	ATOM	4321	O	VAL	B	705	42.930	19.252	62.462	1.00	32.10	B
5	ATOM	4322	N	HIS	B	706	44.641	17.890	63.003	1.00	35.60	B
	ATOM	4323	CA	HIS	B	706	43.949	16.665	62.613	1.00	37.51	B
	ATOM	4324	CB	HIS	B	706	44.515	16.131	61.302	1.00	40.51	B
	ATOM	4325	CG	HIS	B	706	44.191	16.972	60.110	1.00	43.09	B
10	ATOM	4326	CD2	HIS	B	706	44.947	17.845	59.402	1.00	44.48	B
	ATOM	4327	ND1	HIS	B	706	42.946	16.973	59.521	1.00	43.58	B
	ATOM	4328	CE1	HIS	B	706	42.948	17.814	58.501	1.00	44.83	B
	ATOM	4329	NE2	HIS	B	706	44.149	18.357	58.407	1.00	45.93	B
	ATOM	4330	C	HIS	B	706	44.109	15.583	63.676	1.00	37.67	B
	ATOM	4331	O	HIS	B	706	45.189	15.396	64.267	1.00	38.10	B
15	ATOM	4332	N	ALA	B	707	43.032	14.852	63.917	1.00	37.33	B
	ATOM	4333	CA	ALA	B	707	43.104	13.773	64.891	1.00	35.31	B
	ATOM	4334	CB	ALA	B	707	42.368	14.163	66.163	1.00	33.61	B
	ATOM	4335	C	ALA	B	707	42.540	12.479	64.322	1.00	33.93	B
	ATOM	4336	O	ALA	B	707	42.616	11.455	64.979	1.00	33.97	B
20	ATOM	4337	N	ASN	B	708	42.000	12.508	63.103	1.00	32.93	B
	ATOM	4338	CA	ASN	B	708	41.438	11.278	62.566	1.00	32.08	B
	ATOM	4339	CB	ASN	B	708	39.900	11.381	62.527	1.00	30.21	B
	ATOM	4340	CG	ASN	B	708	39.282	11.431	63.935	1.00	29.73	B
	ATOM	4341	OD1	ASN	B	708	39.641	10.644	64.808	1.00	32.17	B
25	ATOM	4342	ND2	ASN	B	708	38.369	12.355	64.155	1.00	27.91	B
	ATOM	4343	C	ASN	B	708	41.998	10.810	61.227	1.00	31.64	B
	ATOM	4344	O	ASN	B	708	41.468	9.888	60.605	1.00	30.96	B
	ATOM	4345	N	ILE	B	709	43.104	11.412	60.803	1.00	31.19	B
	ATOM	4346	CA	ILE	B	709	43.709	11.050	59.526	1.00	29.76	B
30	ATOM	4347	CB	ILE	B	709	45.027	11.813	59.279	1.00	30.79	B
	ATOM	4348	CG2	ILE	B	709	45.414	11.698	57.830	1.00	30.87	B
	ATOM	4349	CG1	ILE	B	709	44.846	13.292	59.585	1.00	31.89	B
	ATOM	4350	CD1	ILE	B	709	43.831	13.966	58.690	1.00	33.84	B
	ATOM	4351	C	ILE	B	709	43.992	9.554	59.404	1.00	27.56	B
35	ATOM	4352	O	ILE	B	709	43.923	9.003	58.316	1.00	28.85	B
	ATOM	4353	N	LEU	B	710	44.335	8.892	60.498	1.00	24.88	B
	ATOM	4354	CA	LEU	B	710	44.600	7.464	60.406	1.00	23.14	B
	ATOM	4355	CB	LEU	B	710	46.101	7.207	60.581	1.00	19.23	B
	ATOM	4356	CG	LEU	B	710	47.171	7.770	59.617	1.00	17.21	B
40	ATOM	4357	CD1	LEU	B	710	48.565	7.336	60.119	1.00	12.65	B
	ATOM	4358	CD2	LEU	B	710	46.952	7.271	58.159	1.00	11.32	B
	ATOM	4359	C	LEU	B	710	43.787	6.738	61.491	1.00	24.82	B
	ATOM	4360	O	LEU	B	710	44.278	5.820	62.165	1.00	26.12	B
	ATOM	4361	N	LYS	B	711	42.540	7.172	61.668	1.00	24.22	B
45	ATOM	4362	CA	LYS	B	711	41.672	6.583	62.678	1.00	23.87	B
	ATOM	4363	CB	LYS	B	711	40.223	7.113	62.551	1.00	23.07	B
	ATOM	4364	CG	LYS	B	711	39.704	7.286	61.127	0.00	24.07	B
	ATOM	4365	CD	LYS	B	711	39.138	6.000	60.567	0.00	24.51	B
	ATOM	4366	CE	LYS	B	711	38.815	6.171	59.096	0.00	24.91	B
50	ATOM	4367	NZ	LYS	B	711	38.073	5.005	58.557	0.00	25.25	B
	ATOM	4368	C	LYS	B	711	41.697	5.066	62.640	1.00	22.54	B
	ATOM	4369	O	LYS	B	711	41.789	4.435	63.682	1.00	21.78	B
	ATOM	4370	N	ASP	B	712	41.656	4.474	61.450	1.00	24.59	B
	ATOM	4371	CA	ASP	B	712	41.649	3.009	61.346	1.00	26.66	B

	ATOM	4372	CB	ASP	B	712	41.358	2.577	59.902	1.00	27.40	B
	ATOM	4373	CG	ASP	B	712	42.533	2.779	58.971	1.00	29.97	B
	ATOM	4374	OD1	ASP	B	712	43.376	3.660	59.238	1.00	31.04	B
	ATOM	4375	OD2	ASP	B	712	42.601	2.059	57.945	1.00	32.95	B
5	ATOM	4376	C	ASP	B	712	42.908	2.320	61.846	1.00	27.18	B
	ATOM	4377	O	ASP	B	712	42.933	1.100	61.992	1.00	28.41	B
	ATOM	4378	N	ALA	B	713	43.943	3.099	62.131	1.00	26.51	B
	ATOM	4379	CA	ALA	B	713	45.192	2.526	62.600	1.00	27.91	B
	ATOM	4380	CB	ALA	B	713	46.334	3.505	62.337	1.00	25.17	B
10	ATOM	4381	C	ALA	B	713	45.117	2.185	64.091	1.00	29.57	B
	ATOM	4382	O	ALA	B	713	44.650	3.003	64.889	1.00	30.09	B
	ATOM	4383	N	ASP	B	714	45.584	0.991	64.467	1.00	30.92	B
	ATOM	4384	CA	ASP	B	714	45.568	0.564	65.873	1.00	33.02	B
	ATOM	4385	CB	ASP	B	714	45.300	-0.947	65.975	1.00	34.69	B
15	ATOM	4386	CG	ASP	B	714	43.997	-1.348	65.333	1.00	36.43	B
	ATOM	4387	OD1	ASP	B	714	42.933	-0.920	65.810	1.00	38.16	B
	ATOM	4388	OD2	ASP	B	714	44.033	-2.089	64.337	1.00	40.68	B
	ATOM	4389	C	ASP	B	714	46.871	0.908	66.620	1.00	33.35	B
	ATOM	4390	O	ASP	B	714	46.871	1.124	67.837	1.00	33.65	B
20	ATOM	4391	N	GLN	B	715	47.979	0.948	65.888	1.00	32.50	B
	ATOM	4392	CA	GLN	B	715	49.272	1.292	66.470	1.00	31.33	B
	ATOM	4393	CB	GLN	B	715	50.053	0.028	66.851	1.00	32.90	B
	ATOM	4394	CG	GLN	B	715	49.555	-0.657	68.107	1.00	36.42	B
	ATOM	4395	CD	GLN	B	715	49.806	0.172	69.355	1.00	39.19	B
25	ATOM	4396	OE1	GLN	B	715	49.528	-0.273	70.465	1.00	39.45	B
	ATOM	4397	NE2	GLN	B	715	50.342	1.389	69.175	1.00	41.12	B
	ATOM	4398	C	GLN	B	715	50.063	2.123	65.465	1.00	29.87	B
	ATOM	4399	O	GLN	B	715	49.897	1.967	64.254	1.00	28.89	B
	ATOM	4400	N	ILE	B	716	50.885	3.038	65.968	1.00	28.35	B
30	ATOM	4401	CA	ILE	B	716	51.712	3.875	65.102	1.00	26.58	B
	ATOM	4402	CB	ILE	B	716	51.360	5.388	65.216	1.00	26.71	B
	ATOM	4403	CG2	ILE	B	716	52.387	6.226	64.452	1.00	24.23	B
	ATOM	4404	CG1	ILE	B	716	49.979	5.655	64.611	1.00	27.09	B
	ATOM	4405	CD1	ILE	B	716	48.830	5.042	65.381	1.00	29.06	B
35	ATOM	4406	C	ILE	B	716	53.137	3.644	65.567	1.00	26.24	B
	ATOM	4407	O	ILE	B	716	53.563	4.184	66.583	1.00	25.69	B
	ATOM	4408	N	TRP	B	717	53.870	2.833	64.818	1.00	25.09	B
	ATOM	4409	CA	TRP	B	717	55.219	2.505	65.198	1.00	25.49	B
	ATOM	4410	CB	TRP	B	717	55.658	1.210	64.497	1.00	28.30	B
40	ATOM	4411	CG	TRP	B	717	54.780	0.010	64.877	1.00	31.04	B
	ATOM	4412	CD2	TRP	B	717	54.454	-0.438	66.203	1.00	29.45	B
	ATOM	4413	CE2	TRP	B	717	53.559	-1.521	66.071	1.00	29.85	B
	ATOM	4414	CE3	TRP	B	717	54.828	-0.029	67.483	1.00	30.32	B
	ATOM	4415	CD1	TRP	B	717	54.091	-0.807	64.024	1.00	30.88	B
45	ATOM	4416	NE1	TRP	B	717	53.353	-1.724	64.736	1.00	29.32	B
	ATOM	4417	CZ2	TRP	B	717	53.027	-2.199	67.172	1.00	33.01	B
	ATOM	4418	CZ3	TRP	B	717	54.295	-0.706	68.583	1.00	33.00	B
	ATOM	4419	CH2	TRP	B	717	53.406	-1.778	68.416	1.00	32.26	B
	ATOM	4420	C	TRP	B	717	56.207	3.611	64.925	1.00	25.13	B
50	ATOM	4421	O	TRP	B	717	56.995	3.961	65.782	1.00	27.18	B
	ATOM	4422	N	SER	B	718	56.163	4.189	63.743	1.00	24.84	B
	ATOM	4423	CA	SER	B	718	57.127	5.212	63.423	1.00	24.34	B
	ATOM	4424	CB	SER	B	718	58.314	4.536	62.727	1.00	24.77	B
	ATOM	4425	OG	SER	B	718	59.315	5.464	62.352	1.00	29.36	B

	ATOM	4426	C	SER	B	718	56.477	6.265	62.533	1.00	23.95	B
	ATOM	4427	O	SER	B	718	55.668	5.949	61.663	1.00	24.34	B
	ATOM	4428	N	VAL	B	719	56.813	7.521	62.754	1.00	21.34	B
	ATOM	4429	CA	VAL	B	719	56.236	8.549	61.934	1.00	20.74	B
5	ATOM	4430	CB	VAL	B	719	55.041	9.202	62.663	1.00	20.34	B
	ATOM	4431	CG1	VAL	B	719	55.531	10.069	63.799	1.00	20.79	B
	ATOM	4432	CG2	VAL	B	719	54.182	9.964	61.685	1.00	20.98	B
	ATOM	4433	C	VAL	B	719	57.355	9.538	61.608	1.00	21.48	B
	ATOM	4434	O	VAL	B	719	58.204	9.840	62.452	1.00	21.37	B
10	ATOM	4435	N	ASN	B	720	57.391	10.001	60.368	1.00	20.75	B
	ATOM	4436	CA	ASN	B	720	58.434	10.915	59.950	1.00	20.33	B
	ATOM	4437	CB	ASN	B	720	59.582	10.130	59.331	1.00	19.95	B
	ATOM	4438	CG	ASN	B	720	60.744	11.013	58.939	1.00	20.71	B
	ATOM	4439	OD1	ASN	B	720	60.570	12.186	58.613	1.00	22.75	B
15	ATOM	4440	ND2	ASN	B	720	61.934	10.452	58.960	1.00	19.81	B
	ATOM	4441	C	ASN	B	720	57.831	11.792	58.885	1.00	21.17	B
	ATOM	4442	O	ASN	B	720	57.037	11.318	58.078	1.00	23.00	B
	ATOM	4443	N	PHE	B	721	58.187	13.067	58.850	1.00	20.66	B
	ATOM	4444	CA	PHE	B	721	57.630	13.907	57.791	1.00	21.75	B
20	ATOM	4445	CB	PHE	B	721	56.339	14.591	58.289	1.00	17.46	B
	ATOM	4446	CG	PHE	B	721	56.556	15.653	59.312	1.00	14.32	B
	ATOM	4447	CD1	PHE	B	721	56.870	16.939	58.921	1.00	10.85	B
	ATOM	4448	CD2	PHE	B	721	56.404	15.387	60.660	1.00	11.84	B
	ATOM	4449	CE1	PHE	B	721	57.028	17.953	59.855	1.00	10.06	B
25	ATOM	4450	CE2	PHE	B	721	56.561	16.405	61.607	1.00	13.14	B
	ATOM	4451	CZ	PHE	B	721	56.873	17.693	61.198	1.00	12.02	B
	ATOM	4452	C	PHE	B	721	58.656	14.902	57.259	1.00	22.48	B
	ATOM	4453	O	PHE	B	721	59.528	15.344	58.000	1.00	21.67	B
	ATOM	4454	N	LYS	B	722	58.584	15.205	55.961	1.00	24.01	B
30	ATOM	4455	CA	LYS	B	722	59.508	16.161	55.320	1.00	24.93	B
	ATOM	4456	CB	LYS	B	722	60.752	15.450	54.783	1.00	25.59	B
	ATOM	4457	CG	LYS	B	722	61.838	15.134	55.800	1.00	27.22	B
	ATOM	4458	CD	LYS	B	722	62.834	16.283	55.958	0.00	27.08	B
	ATOM	4459	CE	LYS	B	722	62.210	17.519	56.576	0.00	27.46	B
35	ATOM	4460	NZ	LYS	B	722	63.225	18.601	56.697	0.00	27.62	B
	ATOM	4461	C	LYS	B	722	58.838	16.863	54.151	1.00	24.47	B
	ATOM	4462	O	LYS	B	722	58.571	16.242	53.121	1.00	25.21	B
	ATOM	4463	N	GLY	B	723	58.569	18.153	54.298	1.00	24.23	B
	ATOM	4464	CA	GLY	B	723	57.937	18.872	53.209	1.00	26.31	B
40	ATOM	4465	C	GLY	B	723	56.464	18.536	53.019	1.00	28.74	B
	ATOM	4466	O	GLY	B	723	55.694	18.529	53.979	1.00	29.75	B
	ATOM	4467	N	LYS	B	724	56.057	18.235	51.794	1.00	28.84	B
	ATOM	4468	CA	LYS	B	724	54.652	17.941	51.530	1.00	29.80	B
	ATOM	4469	CB	LYS	B	724	54.352	18.219	50.074	1.00	31.52	B
45	ATOM	4470	CG	LYS	B	724	55.436	17.698	49.171	1.00	32.34	B
	ATOM	4471	CD	LYS	B	724	54.881	16.783	48.115	1.00	33.78	B
	ATOM	4472	CE	LYS	B	724	55.974	16.447	47.107	1.00	35.08	B
	ATOM	4473	NZ	LYS	B	724	56.379	17.659	46.344	1.00	33.47	B
	ATOM	4474	C	LYS	B	724	54.184	16.535	51.841	1.00	29.68	B
50	ATOM	4475	O	LYS	B	724	52.988	16.260	51.801	1.00	28.58	B
	ATOM	4476	N	THR	B	725	55.121	15.643	52.135	1.00	29.01	B
	ATOM	4477	CA	THR	B	725	54.768	14.261	52.412	1.00	28.07	B
	ATOM	4478	CB	THR	B	725	55.459	13.315	51.372	1.00	28.24	B
	ATOM	4479	OG1	THR	B	725	55.740	12.040	51.957	1.00	28.44	B

	ATOM	4480	CG2	THR	B	725	56.732	13.943	50.850	1.00	29.05	B
	ATOM	4481	C	THR	B	725	55.081	13.853	53.847	1.00	27.60	B
	ATOM	4482	O	THR	B	725	56.070	14.292	54.445	1.00	27.85	B
	ATOM	4483	N	LEU	B	726	54.190	13.036	54.399	1.00	26.00	B
5	ATOM	4484	CA	LEU	B	726	54.310	12.528	55.755	1.00	24.86	B
	ATOM	4485	CB	LEU	B	726	53.147	13.030	56.612	1.00	23.41	B
	ATOM	4486	CG	LEU	B	726	52.907	12.266	57.924	1.00	21.65	B
	ATOM	4487	CD1	LEU	B	726	54.123	12.369	58.805	1.00	24.41	B
	ATOM	4488	CD2	LEU	B	726	51.698	12.816	58.643	1.00	21.21	B
10	ATOM	4489	C	LEU	B	726	54.254	11.014	55.677	1.00	25.90	B
	ATOM	4490	O	LEU	B	726	53.370	10.464	55.019	1.00	27.58	B
	ATOM	4491	N	VAL	B	727	55.196	10.329	56.315	1.00	24.78	B
	ATOM	4492	CA	VAL	B	727	55.151	8.875	56.283	1.00	25.06	B
	ATOM	4493	CB	VAL	B	727	56.388	8.256	55.556	1.00	23.86	B
15	ATOM	4494	CG1	VAL	B	727	56.432	8.730	54.129	1.00	22.56	B
	ATOM	4495	CG2	VAL	B	727	57.678	8.571	56.296	1.00	23.51	B
	ATOM	4496	C	VAL	B	727	55.009	8.257	57.680	1.00	25.61	B
	ATOM	4497	O	VAL	B	727	55.637	8.717	58.641	1.00	25.40	B
	ATOM	4498	N	ALA	B	728	54.163	7.224	57.775	1.00	26.51	B
20	ATOM	4499	CA	ALA	B	728	53.898	6.501	59.028	1.00	27.01	B
	ATOM	4500	CB	ALA	B	728	52.656	7.087	59.692	1.00	25.86	B
	ATOM	4501	C	ALA	B	728	53.734	4.960	58.886	1.00	27.72	B
	ATOM	4502	O	ALA	B	728	52.981	4.480	58.039	1.00	28.25	B
	ATOM	4503	N	ALA	B	729	54.457	4.204	59.718	1.00	29.53	B
25	ATOM	4504	CA	ALA	B	729	54.401	2.735	59.745	1.00	30.38	B
	ATOM	4505	CB	ALA	B	729	55.761	2.150	60.042	1.00	26.88	B
	ATOM	4506	C	ALA	B	729	53.441	2.404	60.876	1.00	32.48	B
	ATOM	4507	O	ALA	B	729	53.692	2.754	62.036	1.00	32.95	B
	ATOM	4508	N	VAL	B	730	52.358	1.710	60.541	1.00	34.76	B
30	ATOM	4509	CA	VAL	B	730	51.326	1.409	61.520	1.00	36.48	B
	ATOM	4510	CB	VAL	B	730	50.133	2.339	61.277	1.00	35.80	B
	ATOM	4511	CG1	VAL	B	730	50.546	3.802	61.484	1.00	35.67	B
	ATOM	4512	CG2	VAL	B	730	49.642	2.148	59.859	1.00	35.12	B
	ATOM	4513	C	VAL	B	730	50.819	-0.022	61.471	1.00	37.73	B
35	ATOM	4514	O	VAL	B	730	51.069	-0.738	60.507	1.00	39.94	B
	ATOM	4515	N	GLU	B	731	50.102	-0.422	62.520	1.00	38.43	B
	ATOM	4516	CA	GLU	B	731	49.509	-1.755	62.608	1.00	38.21	B
	ATOM	4517	CB	GLU	B	731	49.851	-2.413	63.929	1.00	37.52	B
	ATOM	4518	CG	GLU	B	731	49.515	-3.869	63.933	1.00	39.46	B
40	ATOM	4519	CD	GLU	B	731	49.255	-4.398	65.328	1.00	41.40	B
	ATOM	4520	OE1	GLU	B	731	48.163	-4.105	65.873	1.00	41.33	B
	ATOM	4521	OE2	GLU	B	731	50.140	-5.101	65.877	1.00	42.25	B
	ATOM	4522	C	GLU	B	731	47.996	-1.611	62.504	1.00	39.22	B
	ATOM	4523	O	GLU	B	731	47.393	-0.781	63.189	1.00	38.41	B
45	ATOM	4524	N	LYS	B	732	47.382	-2.424	61.652	1.00	41.10	B
	ATOM	4525	CA	LYS	B	732	45.938	-2.358	61.449	1.00	43.00	B
	ATOM	4526	CB	LYS	B	732	45.635	-1.485	60.226	1.00	42.61	B
	ATOM	4527	CG	LYS	B	732	46.197	-0.077	60.333	0.00	43.37	B
	ATOM	4528	CD	LYS	B	732	46.607	0.492	58.981	0.00	43.64	B
50	ATOM	4529	CE	LYS	B	732	45.431	0.678	58.036	0.00	43.89	B
	ATOM	4530	NZ	LYS	B	732	45.868	1.358	56.783	0.00	44.01	B
	ATOM	4531	C	LYS	B	732	45.381	-3.753	61.237	1.00	44.67	B
	ATOM	4532	O	LYS	B	732	45.879	-4.500	60.393	1.00	45.72	B
	ATOM	4533	N	ASP	B	733	44.350	-4.100	62.004	1.00	46.86	B

	ATOM	4534	CA	ASP	B	733	43.717	-5.417	61.898	1.00	48.20	B
	ATOM	4535	CB	ASP	B	733	43.098	-5.602	60.502	1.00	51.83	B
	ATOM	4536	CG	ASP	B	733	42.192	-6.824	60.411	1.00	54.62	B
	ATOM	4537	OD1	ASP	B	733	42.658	-7.894	59.947	1.00	55.49	B
5	ATOM	4538	OD2	ASP	B	733	41.009	-6.708	60.812	1.00	55.81	B
	ATOM	4539	C	ASP	B	733	44.744	-6.520	62.159	1.00	46.65	B
	ATOM	4540	O	ASP	B	733	44.653	-7.621	61.614	1.00	46.27	B
	ATOM	4541	N	GLY	B	734	45.739	-6.203	62.977	1.00	45.55	B
	ATOM	4542	CA	GLY	B	734	46.749	-7.182	63.308	1.00	45.42	B
10	ATOM	4543	C	GLY	B	734	47.792	-7.446	62.245	1.00	45.85	B
	ATOM	4544	O	GLY	B	734	48.334	-8.548	62.183	1.00	46.44	B
	ATOM	4545	N	GLN	B	735	48.073	-6.454	61.401	1.00	46.81	B
	ATOM	4546	CA	GLN	B	735	49.093	-6.599	60.355	1.00	47.05	B
	ATOM	4547	CB	GLN	B	735	48.461	-7.018	59.028	1.00	48.17	B
15	ATOM	4548	CG	GLN	B	735	48.028	-8.461	59.027	1.00	52.88	B
	ATOM	4549	CD	GLN	B	735	46.961	-8.755	57.990	1.00	56.44	B
	ATOM	4550	OE1	GLN	B	735	46.245	-9.766	58.087	1.00	58.95	B
	ATOM	4551	NE2	GLN	B	735	46.840	-7.878	56.993	1.00	55.74	B
	ATOM	4552	C	GLN	B	735	49.897	-5.317	60.176	1.00	45.22	B
20	ATOM	4553	O	GLN	B	735	49.597	-4.297	60.789	1.00	46.16	B
	ATOM	4554	N	SER	B	736	50.924	-5.394	59.336	1.00	42.48	B
	ATOM	4555	CA	SER	B	736	51.817	-4.278	59.061	1.00	39.38	B
	ATOM	4556	CB	SER	B	736	53.256	-4.791	59.003	1.00	40.16	B
	ATOM	4557	OG	SER	B	736	54.176	-3.797	59.394	1.00	40.72	B
25	ATOM	4558	C	SER	B	736	51.468	-3.563	57.753	1.00	37.61	B
	ATOM	4559	O	SER	B	736	51.155	-4.193	56.734	1.00	37.66	B
	ATOM	4560	N	PHE	B	737	51.549	-2.239	57.797	1.00	33.84	B
	ATOM	4561	CA	PHE	B	737	51.228	-1.405	56.655	1.00	31.74	B
	ATOM	4562	CB	PHE	B	737	49.753	-1.006	56.716	1.00	32.02	B
30	ATOM	4563	CG	PHE	B	737	48.802	-2.099	56.337	1.00	33.36	B
	ATOM	4564	CD1	PHE	B	737	48.776	-2.582	55.041	1.00	34.70	B
	ATOM	4565	CD2	PHE	B	737	47.894	-2.606	57.255	1.00	35.15	B
	ATOM	4566	CE1	PHE	B	737	47.857	-3.545	54.655	1.00	36.59	B
	ATOM	4567	CE2	PHE	B	737	46.964	-3.573	56.878	1.00	35.49	B
35	ATOM	4568	CZ	PHE	B	737	46.946	-4.044	55.573	1.00	36.38	B
	ATOM	4569	C	PHE	B	737	52.077	-0.134	56.644	1.00	30.68	B
	ATOM	4570	O	PHE	B	737	52.650	0.254	57.665	1.00	31.62	B
	ATOM	4571	N	LEU	B	738	52.165	0.510	55.485	1.00	27.59	B
	ATOM	4572	CA	LEU	B	738	52.905	1.758	55.373	1.00	25.56	B
40	ATOM	4573	CB	LEU	B	738	54.042	1.679	54.355	1.00	25.25	B
	ATOM	4574	CG	LEU	B	738	54.884	2.973	54.305	1.00	25.05	B
	ATOM	4575	CD1	LEU	B	738	55.668	3.104	55.614	1.00	22.91	B
	ATOM	4576	CD2	LEU	B	738	55.839	2.973	53.131	1.00	21.80	B
	ATOM	4577	C	LEU	B	738	51.947	2.841	54.922	1.00	24.87	B
45	ATOM	4578	O	LEU	B	738	51.336	2.743	53.864	1.00	23.89	B
	ATOM	4579	N	GLU	B	739	51.820	3.882	55.728	1.00	24.71	B
	ATOM	4580	CA	GLU	B	739	50.940	4.976	55.372	1.00	23.29	B
	ATOM	4581	CB	GLU	B	739	50.206	5.458	56.612	1.00	24.09	B
	ATOM	4582	CG	GLU	B	739	48.692	5.452	56.495	1.00	28.17	B
50	ATOM	4583	CD	GLU	B	739	48.058	4.066	56.517	1.00	28.62	B
	ATOM	4584	OE1	GLU	B	739	48.352	3.273	57.426	1.00	31.20	B
	ATOM	4585	OE2	GLU	B	739	47.232	3.782	55.633	1.00	28.53	B
	ATOM	4586	C	GLU	B	739	51.795	6.094	54.780	1.00	20.71	B
	ATOM	4587	O	GLU	B	739	52.906	6.329	55.235	1.00	20.52	B

	ATOM	4588	N	ILE	B	740	51.290	6.740	53.732	1.00	19.91	B
	ATOM	4589	CA	ILE	B	740	51.968	7.868	53.075	1.00	19.31	B
	ATOM	4590	CB	ILE	B	740	52.572	7.473	51.720	1.00	17.66	B
	ATOM	4591	CG2	ILE	B	740	53.171	8.701	51.030	1.00	15.65	B
5	ATOM	4592	CG1	ILE	B	740	53.604	6.379	51.926	1.00	16.52	B
	ATOM	4593	CD1	ILE	B	740	54.155	5.833	50.629	1.00	18.73	B
	ATOM	4594	C	ILE	B	740	50.891	8.923	52.849	1.00	19.07	B
	ATOM	4595	O	ILE	B	740	49.886	8.655	52.209	1.00	19.78	B
	ATOM	4596	N	LEU	B	741	51.106	10.111	53.395	1.00	19.72	B
10	ATOM	4597	CA	LEU	B	741	50.151	11.188	53.259	1.00	21.30	B
	ATOM	4598	CB	LEU	B	741	49.728	11.648	54.645	1.00	22.07	B
	ATOM	4599	CG	LEU	B	741	49.077	10.572	55.530	1.00	23.25	B
	ATOM	4600	CD1	LEU	B	741	48.660	11.188	56.855	1.00	23.41	B
	ATOM	4601	CD2	LEU	B	741	47.856	9.989	54.825	1.00	23.48	B
15	ATOM	4602	C	LEU	B	741	50.732	12.357	52.461	1.00	22.75	B
	ATOM	4603	O	LEU	B	741	51.891	12.745	52.656	1.00	24.38	B
	ATOM	4604	N	ASP	B	742	49.918	12.918	51.571	1.00	23.48	B
	ATOM	4605	CA	ASP	B	742	50.324	14.032	50.711	1.00	24.55	B
	ATOM	4606	CB	ASP	B	742	49.931	13.723	49.276	1.00	26.67	B
20	ATOM	4607	CG	ASP	B	742	50.733	14.515	48.271	1.00	28.63	B
	ATOM	4608	OD1	ASP	B	742	50.840	15.760	48.424	1.00	28.82	B
	ATOM	4609	OD2	ASP	B	742	51.245	13.879	47.328	1.00	28.63	B
	ATOM	4610	C	ASP	B	742	49.688	15.363	51.103	1.00	25.06	B
	ATOM	4611	O	ASP	B	742	48.481	15.436	51.305	1.00	26.84	B
25	ATOM	4612	N	PHE	B	743	50.484	16.423	51.183	1.00	25.71	B
	ATOM	4613	CA	PHE	B	743	49.943	17.731	51.558	1.00	27.52	B
	ATOM	4614	CB	PHE	B	743	50.486	18.191	52.912	1.00	26.16	B
	ATOM	4615	CG	PHE	B	743	49.997	17.388	54.073	1.00	24.94	B
	ATOM	4616	CD1	PHE	B	743	50.565	16.158	54.378	1.00	24.17	B
30	ATOM	4617	CD2	PHE	B	743	48.980	17.887	54.890	1.00	23.91	B
	ATOM	4618	CE1	PHE	B	743	50.132	15.437	55.490	1.00	24.90	B
	ATOM	4619	CE2	PHE	B	743	48.537	17.184	56.000	1.00	21.83	B
	ATOM	4620	CZ	PHE	B	743	49.111	15.957	56.306	1.00	23.09	B
	ATOM	4621	C	PHE	B	743	50.249	18.808	50.530	1.00	29.26	B
35	ATOM	4622	O	PHE	B	743	50.140	20.005	50.808	1.00	29.97	B
	ATOM	4623	N	SER	B	744	50.646	18.372	49.344	1.00	30.92	B
	ATOM	4624	CA	SER	B	744	50.955	19.277	48.245	1.00	32.47	B
	ATOM	4625	CB	SER	B	744	51.761	18.531	47.188	1.00	32.25	B
	ATOM	4626	OG	SER	B	744	51.080	17.346	46.824	1.00	29.83	B
40	ATOM	4627	C	SER	B	744	49.649	19.790	47.629	1.00	34.01	B
	ATOM	4628	O	SER	B	744	49.524	21.028	47.432	1.00	35.67	B
	ATOM	4629	OXT	SER	B	744	48.778	18.934	47.348	1.00	33.32	B
	ATOM	4630	CB	SER	C	2	79.559	36.638	46.340	1.00	43.57	C
	ATOM	4631	OG	SER	C	2	79.993	37.690	45.505	1.00	44.36	C
45	ATOM	4632	C	SER	C	2	78.062	35.376	44.763	1.00	44.40	C
	ATOM	4633	O	SER	C	2	78.864	34.452	44.588	1.00	45.41	C
	ATOM	4634	N	SER	C	2	77.555	35.428	47.144	1.00	45.64	C
	ATOM	4635	CA	SER	C	2	78.115	36.241	46.021	1.00	44.62	C
	ATOM	4636	N	ASN	C	3	77.108	35.678	43.890	1.00	43.20	C
50	ATOM	4637	CA	ASN	C	3	76.921	34.908	42.666	1.00	41.97	C
	ATOM	4638	CB	ASN	C	3	75.435	34.551	42.505	1.00	43.04	C
	ATOM	4639	CG	ASN	C	3	74.952	33.552	43.535	1.00	43.55	C
	ATOM	4640	OD1	ASN	C	3	75.330	32.375	43.512	1.00	43.93	C
	ATOM	4641	ND2	ASN	C	3	74.105	34.017	44.448	1.00	43.67	C

	ATOM	4642	C	ASN	C	3	77.392	35.617	41.399	1.00	40.54	C
	ATOM	4643	O	ASN	C	3	77.723	36.800	41.401	1.00	40.39	C
	ATOM	4644	N	VAL	C	4	77.408	34.868	40.306	1.00	39.54	C
	ATOM	4645	CA	VAL	C	4	77.794	35.409	39.014	1.00	37.85	C
5	ATOM	4646	CB	VAL	C	4	79.259	35.135	38.677	1.00	37.25	C
	ATOM	4647	CG1	VAL	C	4	80.128	36.252	39.212	1.00	37.46	C
	ATOM	4648	CG2	VAL	C	4	79.678	33.798	39.261	1.00	36.73	C
	ATOM	4649	C	VAL	C	4	76.959	34.717	37.975	1.00	36.19	C
	ATOM	4650	O	VAL	C	4	76.617	33.547	38.128	1.00	37.44	C
10	ATOM	4651	N	VAL	C	5	76.627	35.440	36.917	1.00	33.92	C
	ATOM	4652	CA	VAL	C	5	75.844	34.864	35.846	1.00	31.07	C
	ATOM	4653	CB	VAL	C	5	74.812	35.871	35.315	1.00	29.79	C
	ATOM	4654	CG1	VAL	C	5	74.186	35.342	34.041	1.00	30.11	C
	ATOM	4655	CG2	VAL	C	5	73.735	36.100	36.359	1.00	28.61	C
15	ATOM	4656	C	VAL	C	5	76.731	34.410	34.693	1.00	29.84	C
	ATOM	4657	O	VAL	C	5	77.601	35.147	34.233	1.00	29.90	C
	ATOM	4658	N	LEU	C	6	76.513	33.177	34.251	1.00	29.14	C
	ATOM	4659	CA	LEU	C	6	77.236	32.597	33.116	1.00	28.08	C
	ATOM	4660	CB	LEU	C	6	77.863	31.253	33.510	1.00	27.11	C
20	ATOM	4661	CG	LEU	C	6	78.872	31.221	34.675	1.00	24.97	C
	ATOM	4662	CD1	LEU	C	6	79.528	29.845	34.700	1.00	24.15	C
	ATOM	4663	CD2	LEU	C	6	79.919	32.293	34.529	1.00	22.63	C
	ATOM	4664	C	LEU	C	6	76.201	32.405	31.990	1.00	27.51	C
	ATOM	4665	O	LEU	C	6	75.218	31.673	32.139	1.00	26.06	C
25	ATOM	4666	N	VAL	C	7	76.422	33.083	30.869	1.00	28.04	C
	ATOM	4667	CA	VAL	C	7	75.498	33.035	29.732	1.00	29.08	C
	ATOM	4668	CB	VAL	C	7	75.410	34.425	29.046	1.00	30.10	C
	ATOM	4669	CG1	VAL	C	7	74.517	34.349	27.805	1.00	30.31	C
	ATOM	4670	CG2	VAL	C	7	74.887	35.454	30.033	1.00	28.75	C
30	ATOM	4671	C	VAL	C	7	75.861	31.988	28.678	1.00	29.01	C
	ATOM	4672	O	VAL	C	7	77.008	31.913	28.226	1.00	28.23	C
	ATOM	4673	N	SER	C	8	74.865	31.191	28.291	1.00	28.51	C
	ATOM	4674	CA	SER	C	8	75.063	30.147	27.296	1.00	27.88	C
	ATOM	4675	CB	SER	C	8	74.009	29.037	27.418	1.00	28.20	C
35	ATOM	4676	OG	SER	C	8	72.804	29.396	26.748	1.00	25.94	C
	ATOM	4677	C	SER	C	8	74.965	30.741	25.898	1.00	28.40	C
	ATOM	4678	O	SER	C	8	74.359	31.803	25.707	1.00	27.07	C
	ATOM	4679	N	GLY	C	9	75.574	30.034	24.941	1.00	27.46	C
	ATOM	4680	CA	GLY	C	9	75.569	30.450	23.553	1.00	26.64	C
40	ATOM	4681	C	GLY	C	9	74.142	30.602	23.067	1.00	26.05	C
	ATOM	4682	O	GLY	C	9	73.874	31.296	22.085	1.00	26.15	C
	ATOM	4683	N	GLU	C	10	73.219	29.941	23.752	1.00	24.38	C
	ATOM	4684	CA	GLU	C	10	71.824	30.034	23.400	1.00	23.90	C
	ATOM	4685	CB	GLU	C	10	71.116	28.716	23.732	1.00	24.63	C
45	ATOM	4686	CG	GLU	C	10	71.338	27.635	22.678	1.00	29.19	C
	ATOM	4687	CD	GLU	C	10	71.102	26.213	23.204	1.00	33.43	C
	ATOM	4688	OE1	GLU	C	10	70.758	25.307	22.400	1.00	35.21	C
	ATOM	4689	OE2	GLU	C	10	71.281	25.992	24.420	1.00	36.33	C
	ATOM	4690	C	GLU	C	10	71.186	31.221	24.133	1.00	23.12	C
50	ATOM	4691	O	GLU	C	10	69.975	31.374	24.128	1.00	20.55	C
	ATOM	4692	N	GLY	C	11	72.008	32.064	24.756	1.00	25.05	C
	ATOM	4693	CA	GLY	C	11	71.491	33.228	25.458	1.00	26.75	C
	ATOM	4694	C	GLY	C	11	70.939	33.036	26.861	1.00	29.02	C
	ATOM	4695	O	GLY	C	11	70.676	34.022	27.557	1.00	28.98	C

	ATOM	4696	N	GLU	C	12	70.757	31.782	27.276	1.00	29.73	C
	ATOM	4697	CA	GLU	C	12	70.238	31.469	28.604	1.00	29.91	C
	ATOM	4698	CB	GLU	C	12	69.778	30.009	28.657	1.00	29.67	C
	ATOM	4699	CG	GLU	C	12	68.537	29.805	27.817	1.00	29.78	C
5	ATOM	4700	CD	GLU	C	12	67.792	28.516	28.112	1.00	31.45	C
	ATOM	4701	OE1	GLU	C	12	68.320	27.419	27.801	1.00	31.80	C
	ATOM	4702	OE2	GLU	C	12	66.663	28.603	28.651	1.00	32.30	C
	ATOM	4703	C	GLU	C	12	71.231	31.769	29.730	1.00	31.37	C
	ATOM	4704	O	GLU	C	12	72.364	31.288	29.723	1.00	31.63	C
10	ATOM	4705	N	ARG	C	13	70.793	32.579	30.693	1.00	32.45	C
	ATOM	4706	CA	ARG	C	13	71.642	32.983	31.807	1.00	33.31	C
	ATOM	4707	CB	ARG	C	13	71.215	34.341	32.335	1.00	33.47	C
	ATOM	4708	CG	ARG	C	13	70.328	35.124	31.392	1.00	35.00	C
	ATOM	4709	CD	ARG	C	13	69.909	36.383	32.092	1.00	35.56	C
15	ATOM	4710	NE	ARG	C	13	71.082	37.195	32.375	1.00	39.21	C
	ATOM	4711	CZ	ARG	C	13	71.210	37.997	33.423	1.00	40.03	C
	ATOM	4712	NH1	ARG	C	13	70.231	38.093	34.310	1.00	39.27	C
	ATOM	4713	NH2	ARG	C	13	72.310	38.726	33.566	1.00	40.62	C
	ATOM	4714	C	ARG	C	13	71.607	31.997	32.949	1.00	33.28	C
20	ATOM	4715	O	ARG	C	13	70.534	31.584	33.387	1.00	33.83	C
	ATOM	4716	N	PHE	C	14	72.790	31.626	33.431	1.00	33.28	C
	ATOM	4717	CA	PHE	C	14	72.916	30.692	34.545	1.00	32.01	C
	ATOM	4718	CB	PHE	C	14	73.791	29.488	34.180	1.00	32.03	C
	ATOM	4719	CG	PHE	C	14	73.173	28.552	33.175	1.00	32.79	C
25	ATOM	4720	CD1	PHE	C	14	73.005	28.935	31.850	1.00	33.70	C
	ATOM	4721	CD2	PHE	C	14	72.815	27.256	33.545	1.00	32.47	C
	ATOM	4722	CE1	PHE	C	14	72.491	28.032	30.910	1.00	34.61	C
	ATOM	4723	CE2	PHE	C	14	72.301	26.349	32.620	1.00	30.80	C
	ATOM	4724	CZ	PHE	C	14	72.141	26.731	31.300	1.00	31.82	C
30	ATOM	4725	C	PHE	C	14	73.560	31.394	35.733	1.00	31.30	C
	ATOM	4726	O	PHE	C	14	74.669	31.918	35.633	1.00	30.38	C
	ATOM	4727	N	THR	C	15	72.860	31.403	36.857	1.00	30.28	C
	ATOM	4728	CA	THR	C	15	73.387	32.013	38.066	1.00	29.27	C
	ATOM	4729	CB	THR	C	15	72.253	32.635	38.900	1.00	28.06	C
35	ATOM	4730	OG1	THR	C	15	71.567	33.612	38.111	1.00	27.43	C
	ATOM	4731	CG2	THR	C	15	72.801	33.282	40.158	1.00	25.34	C
	ATOM	4732	C	THR	C	15	74.060	30.925	38.901	1.00	29.98	C
	ATOM	4733	O	THR	C	15	73.521	29.827	39.032	1.00	30.73	C
	ATOM	4734	N	VAL	C	16	75.244	31.211	39.435	1.00	30.04	C
40	ATOM	4735	CA	VAL	C	16	75.943	30.254	40.291	1.00	31.88	C
	ATOM	4736	CB	VAL	C	16	76.853	29.283	39.491	1.00	32.07	C
	ATOM	4737	CG1	VAL	C	16	76.035	28.547	38.455	1.00	35.42	C
	ATOM	4738	CG2	VAL	C	16	77.988	30.034	38.823	1.00	34.64	C
	ATOM	4739	C	VAL	C	16	76.793	30.991	41.327	1.00	32.89	C
45	ATOM	4740	O	VAL	C	16	77.097	32.176	41.168	1.00	32.60	C
	ATOM	4741	N	ASP	C	17	77.170	30.286	42.390	1.00	33.45	C
	ATOM	4742	CA	ASP	C	17	77.976	30.874	43.455	1.00	33.69	C
	ATOM	4743	CB	ASP	C	17	78.117	29.888	44.618	1.00	35.66	C
	ATOM	4744	CG	ASP	C	17	79.027	30.419	45.727	1.00	38.16	C
50	ATOM	4745	OD1	ASP	C	17	78.721	31.520	46.269	1.00	38.20	C
	ATOM	4746	OD2	ASP	C	17	80.037	29.741	46.047	1.00	36.91	C
	ATOM	4747	C	ASP	C	17	79.347	31.221	42.911	1.00	33.45	C
	ATOM	4748	O	ASP	C	17	80.034	30.352	42.391	1.00	32.08	C
	ATOM	4749	N	LYS	C	18	79.768	32.475	43.045	1.00	35.48	C

5	ATOM	4750	CA	LYS	C	18	81.068	32.853	42.495	1.00	39.15	C
	ATOM	4751	CB	LYS	C	18	81.378	34.325	42.766	1.00	40.50	C
	ATOM	4752	CG	LYS	C	18	81.886	34.630	44.144	1.00	45.70	C
	ATOM	4753	CD	LYS	C	18	82.169	36.128	44.285	1.00	48.13	C
	ATOM	4754	CE	LYS	C	18	83.245	36.589	43.318	1.00	48.38	C
	ATOM	4755	NZ	LYS	C	18	84.546	35.898	43.581	1.00	49.06	C
	ATOM	4756	C	LYS	C	18	82.212	31.978	42.993	1.00	38.99	C
	ATOM	4757	O	LYS	C	18	83.109	31.638	42.228	1.00	38.11	C
10	ATOM	4758	N	LYS	C	19	82.177	31.596	44.263	1.00	39.59	C
	ATOM	4759	CA	LYS	C	19	83.232	30.759	44.813	1.00	38.98	C
	ATOM	4760	CB	LYS	C	19	82.940	30.429	46.274	0.00	39.52	C
	ATOM	4761	CG	LYS	C	19	84.077	29.703	46.968	0.00	40.25	C
15	ATOM	4762	CD	LYS	C	19	83.738	29.363	48.404	0.00	40.84	C
	ATOM	4763	CE	LYS	C	19	82.586	28.380	48.468	0.00	41.18	C
	ATOM	4764	NZ	LYS	C	19	82.206	28.077	49.871	0.00	41.44	C
	ATOM	4765	C	LYS	C	19	83.364	29.470	44.010	1.00	38.49	C
	ATOM	4766	O	LYS	C	19	84.475	29.025	43.725	1.00	37.49	C
	ATOM	4767	N	ILE	C	20	82.223	28.877	43.651	1.00	39.86	C
20	ATOM	4768	CA	ILE	C	20	82.167	27.631	42.858	1.00	40.16	C
	ATOM	4769	CB	ILE	C	20	80.725	27.037	42.836	1.00	39.38	C
	ATOM	4770	CG2	ILE	C	20	80.705	25.698	42.109	1.00	38.50	C
	ATOM	4771	CG1	ILE	C	20	80.225	26.858	44.270	1.00	39.70	C
	ATOM	4772	CD1	ILE	C	20	78.801	26.351	44.371	1.00	41.15	C
25	ATOM	4773	C	ILE	C	20	82.588	27.949	41.421	1.00	40.51	C
	ATOM	4774	O	ILE	C	20	83.424	27.272	40.841	1.00	39.84	C
	ATOM	4775	N	ALA	C	21	81.999	28.999	40.865	1.00	41.64	C
	ATOM	4776	CA	ALA	C	21	82.312	29.423	39.524	1.00	43.06	C
	ATOM	4777	CB	ALA	C	21	81.635	30.753	39.229	1.00	43.43	C
	ATOM	4778	C	ALA	C	21	83.818	29.554	39.349	1.00	43.95	C
30	ATOM	4779	O	ALA	C	21	84.353	29.186	38.307	1.00	45.27	C
	ATOM	4780	N	GLU	C	22	84.506	30.090	40.354	1.00	44.60	C
	ATOM	4781	CA	GLU	C	22	85.958	30.254	40.266	1.00	44.95	C
	ATOM	4782	CB	GLU	C	22	86.546	30.773	41.582	1.00	47.05	C
35	ATOM	4783	CG	GLU	C	22	86.200	32.217	41.915	1.00	50.65	C
	ATOM	4784	CD	GLU	C	22	87.063	32.769	43.035	1.00	52.85	C
	ATOM	4785	OE1	GLU	C	22	87.098	32.164	44.125	1.00	54.88	C
	ATOM	4786	OE2	GLU	C	22	87.716	33.809	42.826	1.00	54.85	C
	ATOM	4787	C	GLU	C	22	86.652	28.949	39.898	1.00	43.86	C
40	ATOM	4788	O	GLU	C	22	87.851	28.933	39.637	1.00	43.78	C
	ATOM	4789	N	ARG	C	23	85.912	27.849	39.893	1.00	42.42	C
	ATOM	4790	CA	ARG	C	23	86.498	26.576	39.517	1.00	42.71	C
	ATOM	4791	CB	ARG	C	23	85.442	25.496	39.602	1.00	43.00	C
	ATOM	4792	CG	ARG	C	23	85.870	24.197	39.043	1.00	44.32	C
	ATOM	4793	CD	ARG	C	23	86.100	23.258	40.161	1.00	46.65	C
45	ATOM	4794	NE	ARG	C	23	87.502	23.204	40.508	1.00	47.94	C
	ATOM	4795	CZ	ARG	C	23	87.967	22.532	41.548	1.00	48.45	C
	ATOM	4796	NH1	ARG	C	23	87.122	21.875	42.338	1.00	46.40	C
	ATOM	4797	NH2	ARG	C	23	89.274	22.493	41.768	1.00	50.58	C
	ATOM	4798	C	ARG	C	23	86.956	26.742	38.072	1.00	42.33	C
50	ATOM	4799	O	ARG	C	23	87.703	25.926	37.536	1.00	41.75	C
	ATOM	4800	N	SER	C	24	86.461	27.812	37.458	1.00	42.76	C
	ATOM	4801	CA	SER	C	24	86.773	28.177	36.087	1.00	43.35	C
	ATOM	4802	CB	SER	C	24	85.531	28.757	35.406	1.00	42.29	C
	ATOM	4803	OG	SER	C	24	85.845	29.241	34.116	1.00	39.65	C

	ATOM	4804	C	SER	C	24	87.868	29.235	36.113	1.00	44.08	C
	ATOM	4805	O	SER	C	24	87.591	30.403	36.361	1.00	44.37	C
	ATOM	4806	N	LEU	C	25	89.109	28.830	35.875	1.00	45.48	C
	ATOM	4807	CA	LEU	C	25	90.217	29.773	35.875	1.00	47.35	C
5	ATOM	4808	CB	LEU	C	25	91.490	29.117	35.350	1.00	48.27	C
	ATOM	4809	CG	LEU	C	25	92.107	28.027	36.219	1.00	48.77	C
	ATOM	4810	CD1	LEU	C	25	93.392	27.506	35.595	0.00	48.78	C
	ATOM	4811	CD2	LEU	C	25	92.365	28.610	37.598	1.00	48.53	C
	ATOM	4812	C	LEU	C	25	89.871	30.932	34.979	1.00	48.70	C
10	ATOM	4813	O	LEU	C	25	90.293	32.064	35.233	1.00	48.05	C
	ATOM	4814	N	LEU	C	26	89.116	30.635	33.919	1.00	50.30	C
	ATOM	4815	CA	LEU	C	26	88.703	31.658	32.956	1.00	50.59	C
	ATOM	4816	CB	LEU	C	26	87.901	31.046	31.787	1.00	50.13	C
	ATOM	4817	CG	LEU	C	26	87.543	31.994	30.621	1.00	49.31	C
15	ATOM	4818	CD1	LEU	C	26	88.810	32.356	29.880	1.00	49.37	C
	ATOM	4819	CD2	LEU	C	26	86.542	31.346	29.655	1.00	49.24	C
	ATOM	4820	C	LEU	C	26	87.857	32.687	33.689	1.00	50.59	C
	ATOM	4821	O	LEU	C	26	88.005	33.888	33.478	1.00	50.43	C
	ATOM	4822	N	LEU	C	27	86.980	32.210	34.562	1.00	51.20	C
20	ATOM	4823	CA	LEU	C	27	86.132	33.103	35.325	1.00	53.37	C
	ATOM	4824	CB	LEU	C	27	84.930	32.324	35.871	1.00	54.39	C
	ATOM	4825	CG	LEU	C	27	83.811	33.095	36.583	1.00	55.55	C
	ATOM	4826	CD1	LEU	C	27	84.258	33.408	37.990	1.00	56.54	C
	ATOM	4827	CD2	LEU	C	27	83.445	34.376	35.817	1.00	55.58	C
25	ATOM	4828	C	LEU	C	27	86.947	33.775	36.446	1.00	54.11	C
	ATOM	4829	O	LEU	C	27	86.669	34.918	36.822	1.00	54.13	C
	ATOM	4830	N	LYS	C	28	87.960	33.077	36.961	1.00	54.29	C
	ATOM	4831	CA	LYS	C	28	88.816	33.650	37.993	1.00	54.46	C
	ATOM	4832	CB	LYS	C	28	89.825	32.623	38.506	1.00	54.18	C
30	ATOM	4833	CG	LYS	C	28	89.252	31.586	39.446	1.00	54.09	C
	ATOM	4834	CD	LYS	C	28	90.359	30.727	40.048	0.00	54.84	C
	ATOM	4835	CE	LYS	C	28	91.404	31.584	40.756	0.00	55.16	C
	ATOM	4836	NZ	LYS	C	28	90.817	32.412	41.846	0.00	55.54	C
	ATOM	4837	C	LYS	C	28	89.565	34.851	37.408	1.00	55.03	C
35	ATOM	4838	O	LYS	C	28	89.502	35.943	37.956	1.00	54.89	C
	ATOM	4839	N	ASN	C	29	90.269	34.657	36.295	1.00	56.14	C
	ATOM	4840	CA	ASN	C	29	91.006	35.758	35.671	1.00	57.16	C
	ATOM	4841	CB	ASN	C	29	91.659	35.319	34.354	1.00	57.83	C
	ATOM	4842	CG	ASN	C	29	92.642	34.173	34.532	1.00	58.99	C
40	ATOM	4843	OD1	ASN	C	29	93.170	33.633	33.558	1.00	59.61	C
	ATOM	4844	ND2	ASN	C	29	92.895	33.800	35.776	1.00	59.68	C
	ATOM	4845	C	ASN	C	29	90.071	36.923	35.375	1.00	57.45	C
	ATOM	4846	O	ASN	C	29	90.455	38.079	35.525	1.00	57.22	C
	ATOM	4847	N	TYR	C	30	88.849	36.620	34.943	1.00	57.89	C
45	ATOM	4848	CA	TYR	C	30	87.882	37.664	34.615	1.00	58.66	C
	ATOM	4849	CB	TYR	C	30	86.516	37.039	34.317	1.00	57.87	C
	ATOM	4850	CG	TYR	C	30	85.636	37.872	33.409	1.00	56.71	C
	ATOM	4851	CD1	TYR	C	30	86.054	38.229	32.133	1.00	55.67	C
	ATOM	4852	CE1	TYR	C	30	85.231	38.968	31.282	1.00	55.50	C
50	ATOM	4853	CD2	TYR	C	30	84.373	38.276	33.818	1.00	56.61	C
	ATOM	4854	CE2	TYR	C	30	83.539	39.014	32.979	1.00	56.59	C
	ATOM	4855	CZ	TYR	C	30	83.972	39.355	31.712	1.00	56.92	C
	ATOM	4856	OH	TYR	C	30	83.132	40.065	30.873	1.00	57.63	C
	ATOM	4857	C	TYR	C	30	87.787	38.649	35.783	1.00	60.59	C

5	ATOM	4858	O	TYR	C	30	87.482	39.830	35.590	1.00	59.71	C
	ATOM	4859	N	LEU	C	31	88.062	38.146	36.989	1.00	62.33	C
	ATOM	4860	CA	LEU	C	31	88.047	38.932	38.230	1.00	62.29	C
	ATOM	4861	CB	LEU	C	31	89.371	39.712	38.370	1.00	62.08	C
	ATOM	4862	CG	LEU	C	31	89.853	40.603	37.215	1.00	61.04	C
10	ATOM	4863	CD1	LEU	C	31	89.303	42.000	37.370	1.00	60.84	C
	ATOM	4864	CD2	LEU	C	31	91.363	40.639	37.205	1.00	61.22	C
	ATOM	4865	C	LEU	C	31	86.860	39.875	38.358	1.00	62.55	C
	ATOM	4866	O	LEU	C	31	85.754	39.555	37.917	1.00	63.88	C
	ATOM	4867	N	ILE	C	45	80.545	40.215	37.240	1.00	45.54	C
15	ATOM	4868	CA	ILE	C	45	79.354	39.523	37.719	1.00	45.75	C
	ATOM	4869	CB	ILE	C	45	78.323	40.511	38.318	1.00	46.06	C
	ATOM	4870	CG2	ILE	C	45	77.704	41.376	37.213	1.00	43.89	C
	ATOM	4871	CG1	ILE	C	45	77.248	39.723	39.075	1.00	46.70	C
	ATOM	4872	CD1	ILE	C	45	76.128	40.574	39.614	1.00	48.94	C
20	ATOM	4873	C	ILE	C	45	78.665	38.702	36.617	1.00	45.24	C
	ATOM	4874	O	ILE	C	45	78.069	37.659	36.904	1.00	45.32	C
	ATOM	4875	N	VAL	C	46	78.758	39.158	35.364	1.00	43.40	C
	ATOM	4876	CA	VAL	C	46	78.154	38.438	34.237	1.00	41.39	C
	ATOM	4877	CB	VAL	C	46	76.974	39.226	33.613	1.00	41.64	C
25	ATOM	4878	CG1	VAL	C	46	76.308	38.378	32.531	1.00	41.02	C
	ATOM	4879	CG2	VAL	C	46	75.962	39.604	34.690	1.00	41.38	C
	ATOM	4880	C	VAL	C	46	79.154	38.131	33.123	1.00	39.66	C
	ATOM	4881	O	VAL	C	46	79.480	39.005	32.318	1.00	40.66	C
	ATOM	4882	N	MSE	C	47	79.635	36.892	33.071	1.00	38.75	C
30	ATOM	4883	CA	MSE	C	47	80.597	36.501	32.039	1.00	37.26	C
	ATOM	4884	CB	MSE	C	47	81.753	35.691	32.641	1.00	38.19	C
	ATOM	4885	CG	MSE	C	47	82.901	35.488	31.668	1.00	40.50	C
	ATOM	4886	SE	MSE	C	47	84.215	34.179	32.219	1.00	47.69	C
	ATOM	4887	CE	MSE	C	47	83.332	32.527	31.723	1.00	41.93	C
35	ATOM	4888	C	MSE	C	47	79.924	35.669	30.954	1.00	34.30	C
	ATOM	4889	O	MSE	C	47	79.108	34.793	31.246	1.00	32.32	C
	ATOM	4890	N	PRO	C	48	80.240	35.954	29.682	1.00	32.53	C
	ATOM	4891	CD	PRO	C	48	80.789	37.227	29.204	1.00	31.72	C
	ATOM	4892	CA	PRO	C	48	79.655	35.207	28.566	1.00	32.32	C
40	ATOM	4893	CB	PRO	C	48	79.787	36.176	27.389	1.00	31.12	C
	ATOM	4894	CG	PRO	C	48	79.872	37.514	28.049	1.00	31.73	C
	ATOM	4895	C	PRO	C	48	80.408	33.895	28.302	1.00	31.55	C
	ATOM	4896	O	PRO	C	48	81.615	33.809	28.506	1.00	32.35	C
	ATOM	4897	N	VAL	C	49	79.696	32.864	27.874	1.00	30.22	C
45	ATOM	4898	CA	VAL	C	49	80.347	31.609	27.553	1.00	29.45	C
	ATOM	4899	CB	VAL	C	49	79.832	30.440	28.418	1.00	30.65	C
	ATOM	4900	CG1	VAL	C	49	80.731	29.222	28.234	1.00	29.09	C
	ATOM	4901	CG2	VAL	C	49	79.803	30.851	29.872	1.00	31.28	C
	ATOM	4902	C	VAL	C	49	79.958	31.389	26.105	1.00	28.38	C
50	ATOM	4903	O	VAL	C	49	79.011	30.660	25.798	1.00	28.07	C
	ATOM	4904	N	PRO	C	50	80.673	32.049	25.191	1.00	27.28	C
	ATOM	4905	CD	PRO	C	50	81.736	33.036	25.433	1.00	27.20	C
	ATOM	4906	CA	PRO	C	50	80.410	31.937	23.765	1.00	26.24	C
	ATOM	4907	CB	PRO	C	50	81.504	32.810	23.158	1.00	26.55	C
50	ATOM	4908	CG	PRO	C	50	81.687	33.866	24.182	1.00	25.75	C
	ATOM	4909	C	PRO	C	50	80.426	30.516	23.202	1.00	26.07	C
	ATOM	4910	O	PRO	C	50	81.292	29.698	23.529	1.00	25.12	C
	ATOM	4911	N	ASN	C	51	79.447	30.247	22.347	1.00	25.23	C

	ATOM	4912	CA	ASN	C	51	79.317	28.975	21.668	1.00	25.26	C
	ATOM	4913	CB	ASN	C	51	80.446	28.820	20.660	1.00	26.35	C
	ATOM	4914	CG	ASN	C	51	80.554	30.005	19.737	1.00	27.98	C
	ATOM	4915	OD1	ASN	C	51	79.567	30.413	19.116	1.00	28.79	C
5	ATOM	4916	ND2	ASN	C	51	81.752	30.578	19.644	1.00	27.02	C
	ATOM	4917	C	ASN	C	51	79.299	27.762	22.558	1.00	24.62	C
	ATOM	4918	O	ASN	C	51	80.090	26.861	22.374	1.00	25.28	C
	ATOM	4919	N	VAL	C	52	78.388	27.726	23.510	1.00	25.26	C
	ATOM	4920	CA	VAL	C	52	78.284	26.592	24.395	1.00	25.46	C
10	ATOM	4921	CB	VAL	C	52	78.983	26.866	25.714	1.00	27.00	C
	ATOM	4922	CG1	VAL	C	52	78.759	25.698	26.668	1.00	26.64	C
	ATOM	4923	CG2	VAL	C	52	80.473	27.098	25.487	1.00	27.68	C
	ATOM	4924	C	VAL	C	52	76.808	26.404	24.685	1.00	27.92	C
	ATOM	4925	O	VAL	C	52	76.181	27.275	25.305	1.00	30.25	C
15	ATOM	4926	N	ARG	C	53	76.246	25.278	24.249	1.00	28.81	C
	ATOM	4927	CA	ARG	C	53	74.824	25.012	24.478	1.00	29.52	C
	ATOM	4928	CB	ARG	C	53	74.393	23.688	23.845	1.00	32.39	C
	ATOM	4929	CG	ARG	C	53	74.401	23.661	22.337	1.00	37.27	C
	ATOM	4930	CD	ARG	C	53	73.908	22.307	21.839	1.00	42.50	C
20	ATOM	4931	NE	ARG	C	53	74.746	21.181	22.276	1.00	47.26	C
	ATOM	4932	CZ	ARG	C	53	74.285	20.079	22.871	1.00	49.64	C
	ATOM	4933	NH1	ARG	C	53	72.984	19.945	23.114	1.00	48.76	C
	ATOM	4934	NH2	ARG	C	53	75.126	19.106	23.216	1.00	50.78	C
	ATOM	4935	C	ARG	C	53	74.465	24.959	25.964	1.00	28.83	C
25	ATOM	4936	O	ARG	C	53	75.226	24.471	26.794	1.00	27.65	C
	ATOM	4937	N	SER	C	54	73.274	25.454	26.268	1.00	27.01	C
	ATOM	4938	CA	SER	C	54	72.769	25.467	27.613	1.00	24.06	C
	ATOM	4939	CB	SER	C	54	71.302	25.871	27.612	1.00	22.38	C
	ATOM	4940	OG	SER	C	54	71.159	27.162	27.056	1.00	20.31	C
30	ATOM	4941	C	SER	C	54	72.946	24.093	28.246	1.00	24.61	C
	ATOM	4942	O	SER	C	54	73.676	23.948	29.223	1.00	26.72	C
	ATOM	4943	N	SER	C	55	72.306	23.071	27.698	1.00	23.42	C
	ATOM	4944	CA	SER	C	55	72.455	21.735	28.268	1.00	22.33	C
	ATOM	4945	CB	SER	C	55	71.922	20.684	27.304	1.00	19.49	C
35	ATOM	4946	OG	SER	C	55	72.598	20.765	26.075	1.00	22.52	C
	ATOM	4947	C	SER	C	55	73.909	21.414	28.610	1.00	21.51	C
	ATOM	4948	O	SER	C	55	74.168	20.766	29.613	1.00	23.53	C
	ATOM	4949	N	VAL	C	56	74.851	21.884	27.795	1.00	20.84	C
	ATOM	4950	CA	VAL	C	56	76.274	21.624	28.031	1.00	20.83	C
40	ATOM	4951	CB	VAL	C	56	77.137	21.998	26.757	1.00	20.76	C
	ATOM	4952	CG1	VAL	C	56	78.593	21.624	26.953	1.00	16.97	C
	ATOM	4953	CG2	VAL	C	56	76.583	21.284	25.514	1.00	20.88	C
	ATOM	4954	C	VAL	C	56	76.768	22.418	29.260	1.00	19.61	C
	ATOM	4955	O	VAL	C	56	77.375	21.849	30.172	1.00	18.87	C
45	ATOM	4956	N	LEU	C	57	76.515	23.724	29.271	1.00	19.82	C
	ATOM	4957	CA	LEU	C	57	76.906	24.588	30.379	1.00	20.45	C
	ATOM	4958	CB	LEU	C	57	76.487	26.026	30.075	1.00	17.81	C
	ATOM	4959	CG	LEU	C	57	76.896	27.099	31.084	1.00	15.76	C
	ATOM	4960	CD1	LEU	C	57	78.375	27.066	31.281	1.00	14.13	C
50	ATOM	4961	CD2	LEU	C	57	76.451	28.463	30.589	1.00	17.83	C
	ATOM	4962	C	LEU	C	57	76.231	24.116	31.678	1.00	21.81	C
	ATOM	4963	O	LEU	C	57	76.842	24.076	32.744	1.00	22.15	C
	ATOM	4964	N	GLN	C	58	74.956	23.777	31.588	1.00	22.64	C
	ATOM	4965	CA	GLN	C	58	74.255	23.311	32.757	1.00	24.92	C

	ATOM	4966	CB	GLN	C	58	72.811	22.991	32.418	1.00	25.24	C
	ATOM	4967	CG	GLN	C	58	72.079	22.366	33.567	1.00	27.25	C
	ATOM	4968	CD	GLN	C	58	70.636	22.144	33.271	1.00	28.40	C
	ATOM	4969	OE1	GLN	C	58	70.047	21.177	33.740	1.00	31.18	C
5	ATOM	4970	NE2	GLN	C	58	70.043	23.041	32.500	1.00	29.28	C
	ATOM	4971	C	GLN	C	58	74.938	22.065	33.282	1.00	26.17	C
	ATOM	4972	O	GLN	C	58	75.060	21.872	34.487	1.00	27.72	C
	ATOM	4973	N	LYS	C	59	75.375	21.209	32.373	1.00	27.32	C
	ATOM	4974	CA	LYS	C	59	76.047	19.990	32.771	1.00	29.09	C
10	ATOM	4975	CB	LYS	C	59	76.229	19.093	31.549	1.00	29.32	C
	ATOM	4976	CG	LYS	C	59	76.548	17.651	31.869	1.00	32.80	C
	ATOM	4977	CD	LYS	C	59	75.309	16.788	31.972	1.00	32.66	C
	ATOM	4978	CE	LYS	C	59	75.708	15.346	32.280	1.00	34.41	C
	ATOM	4979	NZ	LYS	C	59	74.566	14.374	32.116	1.00	36.74	C
15	ATOM	4980	C	LYS	C	59	77.406	20.346	33.412	1.00	31.23	C
	ATOM	4981	O	LYS	C	59	77.793	19.750	34.418	1.00	32.05	C
	ATOM	4982	N	VAL	C	60	78.116	21.320	32.837	1.00	31.14	C
	ATOM	4983	CA	VAL	C	60	79.416	21.769	33.350	1.00	30.44	C
	ATOM	4984	CB	VAL	C	60	80.022	22.893	32.461	1.00	30.16	C
20	ATOM	4985	CG1	VAL	C	60	81.236	23.514	33.139	1.00	28.33	C
	ATOM	4986	CG2	VAL	C	60	80.422	22.325	31.109	1.00	32.07	C
	ATOM	4987	C	VAL	C	60	79.310	22.314	34.767	1.00	31.68	C
	ATOM	4988	O	VAL	C	60	80.078	21.953	35.650	1.00	32.71	C
	ATOM	4989	N	ILE	C	61	78.356	23.204	34.969	1.00	32.12	C
25	ATOM	4990	CA	ILE	C	61	78.140	23.804	36.262	1.00	31.24	C
	ATOM	4991	CB	ILE	C	61	77.021	24.824	36.170	1.00	31.54	C
	ATOM	4992	CG2	ILE	C	61	76.601	25.279	37.564	1.00	28.63	C
	ATOM	4993	CG1	ILE	C	61	77.497	25.982	35.297	1.00	31.49	C
	ATOM	4994	CD1	ILE	C	61	76.388	26.850	34.795	1.00	32.68	C
30	ATOM	4995	C	ILE	C	61	77.780	22.749	37.289	1.00	31.52	C
	ATOM	4996	O	ILE	C	61	78.360	22.707	38.368	1.00	31.59	C
	ATOM	4997	N	GLU	C	62	76.836	21.881	36.955	1.00	31.93	C
	ATOM	4998	CA	GLU	C	62	76.443	20.861	37.907	1.00	33.23	C
	ATOM	4999	CB	GLU	C	62	75.295	20.025	37.375	1.00	32.43	C
35	ATOM	5000	CG	GLU	C	62	75.721	18.813	36.636	1.00	34.09	C
	ATOM	5001	CD	GLU	C	62	74.649	17.762	36.649	1.00	35.90	C
	ATOM	5002	OE1	GLU	C	62	74.307	17.292	37.757	1.00	35.78	C
	ATOM	5003	OE2	GLU	C	62	74.143	17.408	35.558	1.00	37.89	C
	ATOM	5004	C	GLU	C	62	77.595	19.939	38.278	1.00	33.56	C
40	ATOM	5005	O	GLU	C	62	77.462	19.096	39.161	1.00	34.70	C
	ATOM	5006	N	TRP	C	63	78.717	20.086	37.593	1.00	33.45	C
	ATOM	5007	CA	TRP	C	63	79.872	19.269	37.888	1.00	33.70	C
	ATOM	5008	CB	TRP	C	63	80.670	18.991	36.622	1.00	33.66	C
	ATOM	5009	CG	TRP	C	63	81.955	18.280	36.884	1.00	33.52	C
45	ATOM	5010	CD2	TRP	C	63	83.211	18.876	37.231	1.00	32.28	C
	ATOM	5011	CE2	TRP	C	63	84.142	17.826	37.386	1.00	32.37	C
	ATOM	5012	CE3	TRP	C	63	83.639	20.196	37.429	1.00	31.95	C
	ATOM	5013	CD1	TRP	C	63	82.167	16.935	36.846	1.00	34.55	C
	ATOM	5014	NE1	TRP	C	63	83.481	16.653	37.143	1.00	34.74	C
50	ATOM	5015	CZ2	TRP	C	63	85.476	18.049	37.726	1.00	32.07	C
	ATOM	5016	CZ3	TRP	C	63	84.965	20.424	37.768	1.00	31.44	C
	ATOM	5017	CH2	TRP	C	63	85.871	19.351	37.914	1.00	32.65	C
	ATOM	5018	C	TRP	C	63	80.726	20.067	38.853	1.00	34.67	C
	ATOM	5019	O	TRP	C	63	81.367	19.512	39.733	1.00	36.11	C

	ATOM	5020	N	ALA	C	64	80.737	21.380	38.686	1.00	36.01	C
	ATOM	5021	CA	ALA	C	64	81.537	22.234	39.551	1.00	38.09	C
	ATOM	5022	CB	ALA	C	64	81.604	23.652	38.975	1.00	38.34	C
	ATOM	5023	C	ALA	C	64	80.954	22.270	40.954	1.00	38.84	C
5	ATOM	5024	O	ALA	C	64	81.653	22.010	41.928	1.00	40.17	C
	ATOM	5025	N	GLU	C	65	79.670	22.605	41.045	1.00	39.31	C
	ATOM	5026	CA	GLU	C	65	78.981	22.675	42.322	1.00	39.42	C
	ATOM	5027	CB	GLU	C	65	77.483	22.928	42.099	1.00	37.23	C
	ATOM	5028	CG	GLU	C	65	77.202	24.210	41.330	1.00	34.34	C
10	ATOM	5029	CD	GLU	C	65	75.724	24.533	41.190	1.00	33.67	C
	ATOM	5030	OE1	GLU	C	65	74.926	23.651	40.805	1.00	33.23	C
	ATOM	5031	OE2	GLU	C	65	75.356	25.688	41.455	1.00	33.33	C
	ATOM	5032	C	GLU	C	65	79.196	21.376	43.101	1.00	41.07	C
	ATOM	5033	O	GLU	C	65	79.379	21.406	44.315	1.00	41.60	C
15	ATOM	5034	N	HIS	C	66	79.190	20.240	42.403	1.00	42.63	C
	ATOM	5035	CA	HIS	C	66	79.391	18.944	43.059	1.00	44.78	C
	ATOM	5036	CB	HIS	C	66	78.988	17.796	42.119	1.00	44.20	C
	ATOM	5037	CG	HIS	C	66	79.334	16.420	42.622	1.00	44.62	C
	ATOM	5038	CD2	HIS	C	66	78.548	15.363	42.937	1.00	43.92	C
20	ATOM	5039	ND1	HIS	C	66	80.634	15.972	42.740	1.00	45.83	C
	ATOM	5040	CE1	HIS	C	66	80.633	14.699	43.095	1.00	43.67	C
	ATOM	5041	NE2	HIS	C	66	79.379	14.305	43.221	1.00	42.62	C
	ATOM	5042	C	HIS	C	66	80.823	18.750	43.544	1.00	46.51	C
	ATOM	5043	O	HIS	C	66	81.063	18.025	44.505	1.00	47.99	C
25	ATOM	5044	N	HIS	C	67	81.781	19.393	42.894	1.00	47.66	C
	ATOM	5045	CA	HIS	C	67	83.163	19.249	43.321	1.00	49.37	C
	ATOM	5046	CB	HIS	C	67	84.059	18.952	42.127	1.00	50.68	C
	ATOM	5047	CG	HIS	C	67	83.964	17.541	41.652	1.00	52.46	C
	ATOM	5048	CD2	HIS	C	67	83.878	16.378	42.337	1.00	53.35	C
30	ATOM	5049	ND1	HIS	C	67	83.926	17.205	40.318	1.00	54.03	C
	ATOM	5050	CE1	HIS	C	67	83.815	15.894	40.199	1.00	53.47	C
	ATOM	5051	NE2	HIS	C	67	83.783	15.369	41.410	1.00	54.73	C
	ATOM	5052	C	HIS	C	67	83.634	20.496	44.013	1.00	50.00	C
	ATOM	5053	O	HIS	C	67	84.831	20.793	44.022	1.00	49.65	C
35	ATOM	5054	N	ARG	C	68	82.685	21.219	44.603	1.00	50.89	C
	ATOM	5055	CA	ARG	C	68	82.996	22.468	45.295	1.00	52.52	C
	ATOM	5056	CB	ARG	C	68	81.721	23.137	45.804	1.00	51.55	C
	ATOM	5057	CG	ARG	C	68	80.882	22.281	46.708	1.00	51.00	C
	ATOM	5058	CD	ARG	C	68	79.609	23.021	47.114	1.00	51.32	C
40	ATOM	5059	NE	ARG	C	68	78.436	22.163	46.984	1.00	50.65	C
	ATOM	5060	CZ	ARG	C	68	78.319	20.978	47.571	1.00	49.83	C
	ATOM	5061	NH1	ARG	C	68	79.299	20.514	48.331	1.00	53.30	C
	ATOM	5062	NH2	ARG	C	68	77.232	20.249	47.391	1.00	50.27	C
	ATOM	5063	C	ARG	C	68	83.967	22.310	46.442	1.00	53.96	C
45	ATOM	5064	O	ARG	C	68	84.685	23.243	46.784	1.00	54.35	C
	ATOM	5065	N	ASP	C	69	83.993	21.134	47.046	1.00	56.66	C
	ATOM	5066	CA	ASP	C	69	84.905	20.921	48.150	1.00	59.49	C
	ATOM	5067	CB	ASP	C	69	84.147	20.357	49.361	1.00	58.83	C
	ATOM	5068	CG	ASP	C	69	82.957	21.232	49.774	1.00	58.82	C
50	ATOM	5069	OD1	ASP	C	69	83.161	22.430	50.067	1.00	57.19	C
	ATOM	5070	OD2	ASP	C	69	81.814	20.718	49.806	1.00	58.80	C
	ATOM	5071	C	ASP	C	69	86.032	19.986	47.722	1.00	61.81	C
	ATOM	5072	O	ASP	C	69	87.029	19.849	48.426	1.00	64.04	C
	ATOM	5073	N	SER	C	70	85.890	19.355	46.561	1.00	62.80	C

	ATOM	5074	CA	SER	C	70	86.928	18.445	46.089	1.00	63.95	C
	ATOM	5075	CB	SER	C	70	86.501	17.796	44.777	1.00	64.08	C
	ATOM	5076	OG	SER	C	70	85.355	16.996	44.990	1.00	65.02	C
	ATOM	5077	C	SER	C	70	88.264	19.161	45.914	1.00	64.84	C
5	ATOM	5078	O	SER	C	70	88.305	20.371	45.697	1.00	65.35	C
	ATOM	5079	N	ASN	C	71	89.360	18.418	46.029	1.00	65.33	C
	ATOM	5080	CA	ASN	C	71	90.678	19.015	45.878	1.00	65.77	C
	ATOM	5081	CB	ASN	C	71	91.549	18.684	47.091	1.00	67.38	C
	ATOM	5082	CG	ASN	C	71	90.805	18.874	48.409	1.00	70.03	C
10	ATOM	5083	OD1	ASN	C	71	90.234	19.943	48.673	1.00	70.29	C
	ATOM	5084	ND2	ASN	C	71	90.807	17.832	49.246	1.00	70.86	C
	ATOM	5085	C	ASN	C	71	91.311	18.488	44.603	1.00	65.48	C
	ATOM	5086	O	ASN	C	71	91.311	17.280	44.351	1.00	65.01	C
	ATOM	5087	N	PHE	C	72	91.830	19.404	43.792	1.00	64.80	C
15	ATOM	5088	CA	PHE	C	72	92.463	19.045	42.529	1.00	64.53	C
	ATOM	5089	CB	PHE	C	72	91.585	19.473	41.342	1.00	60.50	C
	ATOM	5090	CG	PHE	C	72	90.272	18.736	41.247	1.00	55.74	C
	ATOM	5091	CD1	PHE	C	72	89.068	19.433	41.235	1.00	53.23	C
	ATOM	5092	CD2	PHE	C	72	90.238	17.349	41.154	1.00	52.78	C
20	ATOM	5093	CE1	PHE	C	72	87.856	18.758	41.127	1.00	51.24	C
	ATOM	5094	CE2	PHE	C	72	89.027	16.672	41.047	1.00	50.62	C
	ATOM	5095	CZ	PHE	C	72	87.837	17.378	41.034	1.00	50.12	C
	ATOM	5096	C	PHE	C	72	93.818	19.728	42.417	1.00	66.62	C
	ATOM	5097	O	PHE	C	72	93.940	20.918	42.709	1.00	67.09	C
25	ATOM	5098	N	PRO	C	73	94.853	18.981	41.988	1.00	68.12	C
	ATOM	5099	CD	PRO	C	73	94.775	17.557	41.611	1.00	68.63	C
	ATOM	5100	CA	PRO	C	73	96.220	19.493	41.823	1.00	68.91	C
	ATOM	5101	CB	PRO	C	73	96.935	18.342	41.118	1.00	69.55	C
	ATOM	5102	CG	PRO	C	73	96.219	17.133	41.636	1.00	69.28	C
30	ATOM	5103	C	PRO	C	73	96.257	20.778	40.990	1.00	69.17	C
	ATOM	5104	O	PRO	C	73	96.598	21.853	41.487	1.00	69.84	C
	ATOM	5105	N	VAL	C	86	90.900	7.286	36.371	1.00	88.13	C
	ATOM	5106	CA	VAL	C	86	90.597	6.804	37.711	1.00	88.42	C
	ATOM	5107	CB	VAL	C	86	91.894	6.677	38.553	1.00	87.81	C
35	ATOM	5108	CG1	VAL	C	86	92.562	5.342	38.273	0.00	87.97	C
	ATOM	5109	CG2	VAL	C	86	92.855	7.813	38.214	1.00	86.72	C
	ATOM	5110	C	VAL	C	86	89.573	7.685	38.445	1.00	88.62	C
	ATOM	5111	O	VAL	C	86	89.901	8.362	39.423	1.00	88.93	C
	ATOM	5112	N	ASP	C	87	88.328	7.661	37.964	1.00	88.31	C
40	ATOM	5113	CA	ASP	C	87	87.230	8.443	38.547	1.00	87.51	C
	ATOM	5114	CB	ASP	C	87	86.568	9.310	37.475	0.00	88.63	C
	ATOM	5115	CG	ASP	C	87	87.538	10.229	36.783	1.00	89.65	C
	ATOM	5116	OD1	ASP	C	87	87.832	11.313	37.331	1.00	90.42	C
	ATOM	5117	OD2	ASP	C	87	88.011	9.859	35.688	1.00	89.70	C
45	ATOM	5118	C	ASP	C	87	86.150	7.559	39.166	1.00	86.41	C
	ATOM	5119	O	ASP	C	87	86.396	6.413	39.543	0.00	86.24	C
	ATOM	5120	N	SER	C	88	84.944	8.110	39.245	1.00	84.26	C
	ATOM	5121	CA	SER	C	88	83.803	7.402	39.800	1.00	82.05	C
	ATOM	5122	CB	SER	C	88	83.872	7.398	41.324	1.00	81.81	C
50	ATOM	5123	OG	SER	C	88	82.634	6.987	41.874	1.00	81.31	C
	ATOM	5124	C	SER	C	88	82.508	8.067	39.360	1.00	80.69	C
	ATOM	5125	O	SER	C	88	81.919	7.704	38.342	1.00	81.28	C
	ATOM	5126	N	TRP	C	89	82.066	9.042	40.144	1.00	77.91	C
	ATOM	5127	CA	TRP	C	89	80.848	9.780	39.848	1.00	74.10	C

	ATOM	5128	CB	TRP	C	89	80.646	10.859	40.905	1.00	73.48	C
	ATOM	5129	CG	TRP	C	89	79.446	11.708	40.702	1.00	72.20	C
	ATOM	5130	CD2	TRP	C	89	79.428	13.044	40.197	1.00	71.86	C
	ATOM	5131	CE2	TRP	C	89	78.088	13.476	40.209	1.00	71.45	C
5	ATOM	5132	CE3	TRP	C	89	80.418	13.919	39.735	1.00	71.66	C
	ATOM	5133	CD1	TRP	C	89	78.153	11.388	40.988	1.00	71.28	C
	ATOM	5134	NE1	TRP	C	89	77.329	12.446	40.698	1.00	70.67	C
	ATOM	5135	CZ2	TRP	C	89	77.711	14.750	39.780	1.00	71.55	C
	ATOM	5136	CZ3	TRP	C	89	80.043	15.184	39.308	1.00	71.26	C
10	ATOM	5137	CH2	TRP	C	89	78.701	15.587	39.334	1.00	71.21	C
	ATOM	5138	C	TRP	C	89	80.995	10.415	38.473	1.00	72.28	C
	ATOM	5139	O	TRP	C	89	80.021	10.567	37.740	1.00	72.30	C
	ATOM	5140	N	ASP	C	90	82.229	10.779	38.136	1.00	70.00	C
	ATOM	5141	CA	ASP	C	90	82.543	11.389	36.848	1.00	67.79	C
15	ATOM	5142	CB	ASP	C	90	84.011	11.810	36.808	1.00	64.52	C
	ATOM	5143	CG	ASP	C	90	84.300	13.010	37.685	1.00	61.24	C
	ATOM	5144	OD1	ASP	C	90	83.453	13.363	38.530	1.00	59.13	C
	ATOM	5145	OD2	ASP	C	90	85.388	13.594	37.533	1.00	58.53	C
	ATOM	5146	C	ASP	C	90	82.261	10.436	35.691	1.00	67.74	C
20	ATOM	5147	O	ASP	C	90	81.888	10.868	34.597	1.00	68.39	C
	ATOM	5148	N	ARG	C	91	82.460	9.142	35.926	1.00	67.23	C
	ATOM	5149	CA	ARG	C	91	82.197	8.140	34.895	1.00	66.43	C
	ATOM	5150	CB	ARG	C	91	82.671	6.755	35.345	0.00	67.74	C
	ATOM	5151	CG	ARG	C	91	82.250	5.602	34.429	0.00	69.73	C
25	ATOM	5152	CD	ARG	C	91	82.769	5.731	32.997	0.00	71.43	C
	ATOM	5153	NE	ARG	C	91	81.880	6.509	32.132	1.00	73.30	C
	ATOM	5154	CZ	ARG	C	91	81.888	6.448	30.803	1.00	73.96	C
	ATOM	5155	NH1	ARG	C	91	82.739	5.645	30.176	1.00	75.13	C
	ATOM	5156	NH2	ARG	C	91	81.038	7.180	30.098	1.00	73.71	C
30	ATOM	5157	C	ARG	C	91	80.707	8.091	34.580	1.00	64.28	C
	ATOM	5158	O	ARG	C	91	80.322	8.005	33.416	1.00	64.65	C
	ATOM	5159	N	GLU	C	92	79.871	8.156	35.611	1.00	61.21	C
	ATOM	5160	CA	GLU	C	92	78.434	8.111	35.398	1.00	59.24	C
	ATOM	5161	CB	GLU	C	92	77.709	7.733	36.691	1.00	61.28	C
35	ATOM	5162	CG	GLU	C	92	76.200	7.577	36.529	1.00	63.29	C
	ATOM	5163	CD	GLU	C	92	75.816	6.698	35.345	1.00	64.91	C
	ATOM	5164	OE1	GLU	C	92	76.430	5.618	35.171	1.00	65.27	C
	ATOM	5165	OE2	GLU	C	92	74.888	7.087	34.599	1.00	65.86	C
	ATOM	5166	C	GLU	C	92	77.947	9.463	34.908	1.00	56.10	C
40	ATOM	5167	O	GLU	C	92	76.846	9.587	34.379	1.00	55.26	C
	ATOM	5168	N	PHE	C	93	78.786	10.473	35.088	1.00	52.97	C
	ATOM	5169	CA	PHE	C	93	78.470	11.828	34.669	1.00	49.46	C
	ATOM	5170	CB	PHE	C	93	79.271	12.821	35.504	1.00	47.72	C
	ATOM	5171	CG	PHE	C	93	79.168	14.237	35.031	1.00	46.31	C
45	ATOM	5172	CD1	PHE	C	93	77.975	14.936	35.134	1.00	46.80	C
	ATOM	5173	CD2	PHE	C	93	80.274	14.880	34.487	1.00	46.30	C
	ATOM	5174	CE1	PHE	C	93	77.881	16.260	34.698	1.00	46.57	C
	ATOM	5175	CE2	PHE	C	93	80.194	16.200	34.048	1.00	45.89	C
	ATOM	5176	CZ	PHE	C	93	78.995	16.891	34.155	1.00	46.39	C
50	ATOM	5177	C	PHE	C	93	78.805	12.007	33.195	1.00	48.24	C
	ATOM	5178	O	PHE	C	93	78.194	12.829	32.512	1.00	48.29	C
	ATOM	5179	N	LEU	C	94	79.777	11.241	32.706	1.00	46.95	C
	ATOM	5180	CA	LEU	C	94	80.181	11.334	31.304	1.00	46.69	C
	ATOM	5181	CB	LEU	C	94	81.711	11.421	31.201	1.00	43.72	C

	ATOM	5182	CG	LEU	C	94	82.347	12.602	31.931	1.00	42.20	C
	ATOM	5183	CD1	LEU	C	94	83.827	12.571	31.708	1.00	42.01	C
	ATOM	5184	CD2	LEU	C	94	81.761	13.918	31.444	1.00	40.79	C
	ATOM	5185	C	LEU	C	94	79.657	10.163	30.470	1.00	46.61	C
5	ATOM	5186	O	LEU	C	94	80.084	9.950	29.331	1.00	47.53	C
	ATOM	5187	N	LYS	C	95	78.721	9.416	31.044	1.00	46.24	C
	ATOM	5188	CA	LYS	C	95	78.123	8.260	30.382	1.00	46.42	C
	ATOM	5189	CB	LYS	C	95	77.447	7.372	31.436	1.00	48.23	C
	ATOM	5190	CG	LYS	C	95	77.259	5.915	31.045	1.00	48.85	C
10	ATOM	5191	CD	LYS	C	95	75.858	5.649	30.493	1.00	50.94	C
	ATOM	5192	CE	LYS	C	95	74.749	5.845	31.556	1.00	51.20	C
	ATOM	5193	NZ	LYS	C	95	74.537	7.259	32.014	1.00	49.42	C
	ATOM	5194	C	LYS	C	95	77.103	8.758	29.359	1.00	45.40	C
	ATOM	5195	O	LYS	C	95	76.000	8.222	29.234	1.00	45.79	C
15	ATOM	5196	N	VAL	C	96	77.495	9.797	28.631	1.00	42.97	C
	ATOM	5197	CA	VAL	C	96	76.648	10.418	27.627	1.00	39.32	C
	ATOM	5198	CB	VAL	C	96	76.748	11.930	27.759	1.00	38.19	C
	ATOM	5199	CG1	VAL	C	96	76.296	12.335	29.143	1.00	37.83	C
	ATOM	5200	CG2	VAL	C	96	78.182	12.369	27.543	1.00	37.61	C
20	ATOM	5201	C	VAL	C	96	77.069	9.973	26.224	1.00	39.45	C
	ATOM	5202	O	VAL	C	96	77.934	9.110	26.077	1.00	39.51	C
	ATOM	5203	N	ASP	C	97	76.448	10.545	25.197	1.00	38.96	C
	ATOM	5204	CA	ASP	C	97	76.776	10.194	23.820	1.00	38.45	C
	ATOM	5205	CB	ASP	C	97	75.596	10.485	22.907	1.00	40.12	C
25	ATOM	5206	CG	ASP	C	97	75.212	11.951	22.907	1.00	41.57	C
	ATOM	5207	OD1	ASP	C	97	76.061	12.785	23.289	1.00	41.15	C
	ATOM	5208	OD2	ASP	C	97	74.066	12.271	22.516	1.00	42.19	C
	ATOM	5209	C	ASP	C	97	77.986	10.982	23.328	1.00	38.55	C
	ATOM	5210	O	ASP	C	97	78.331	12.014	23.893	1.00	37.77	C
30	ATOM	5211	N	GLN	C	98	78.612	10.505	22.259	1.00	39.05	C
	ATOM	5212	CA	GLN	C	98	79.794	11.157	21.717	1.00	38.40	C
	ATOM	5213	CB	GLN	C	98	80.225	10.485	20.415	1.00	38.10	C
	ATOM	5214	CG	GLN	C	98	80.605	9.023	20.544	1.00	36.09	C
	ATOM	5215	CD	GLN	C	98	81.275	8.497	19.298	1.00	36.91	C
35	ATOM	5216	OE1	GLN	C	98	81.239	9.130	18.236	1.00	36.92	C
	ATOM	5217	NE2	GLN	C	98	81.881	7.324	19.412	1.00	36.42	C
	ATOM	5218	C	GLN	C	98	79.650	12.653	21.470	1.00	39.08	C
	ATOM	5219	O	GLN	C	98	80.599	13.401	21.692	1.00	40.00	C
	ATOM	5220	N	GLU	C	99	78.486	13.088	21.001	1.00	39.22	C
40	ATOM	5221	CA	GLU	C	99	78.271	14.502	20.726	1.00	40.50	C
	ATOM	5222	CB	GLU	C	99	76.891	14.717	20.126	1.00	42.47	C
	ATOM	5223	CG	GLU	C	99	76.918	15.343	18.756	1.00	45.54	C
	ATOM	5224	CD	GLU	C	99	77.806	16.577	18.697	1.00	47.73	C
	ATOM	5225	OE1	GLU	C	99	77.552	17.541	19.462	1.00	47.01	C
45	ATOM	5226	OE2	GLU	C	99	78.757	16.577	17.881	1.00	47.67	C
	ATOM	5227	C	GLU	C	99	78.387	15.335	21.990	1.00	41.46	C
	ATOM	5228	O	GLU	C	99	78.980	16.418	21.993	1.00	41.51	C
	ATOM	5229	N	MSE	C	100	77.788	14.831	23.061	1.00	41.97	C
	ATOM	5230	CA	MSE	C	100	77.818	15.518	24.335	1.00	41.69	C
50	ATOM	5231	CB	MSE	C	100	76.885	14.824	25.333	1.00	45.69	C
	ATOM	5232	CG	MSE	C	100	76.914	15.403	26.735	1.00	51.76	C
	ATOM	5233	SE	MSE	C	100	76.090	17.140	26.925	1.00	62.68	C
	ATOM	5234	CE	MSE	C	100	77.565	18.303	26.510	1.00	57.90	C
	ATOM	5235	C	MSE	C	100	79.243	15.546	24.867	1.00	39.87	C

	ATOM	5236	O	MSE	C	100	79.810	16.626	25.037	1.00	39.79	C
	ATOM	5237	N	LEU	C	101	79.835	14.376	25.115	1.00	37.39	C
	ATOM	5238	CA	LEU	C	101	81.199	14.341	25.651	1.00	34.99	C
	ATOM	5239	CB	LEU	C	101	81.809	12.938	25.539	1.00	33.34	C
5	ATOM	5240	CG	LEU	C	101	83.130	12.730	26.289	1.00	30.53	C
	ATOM	5241	CD1	LEU	C	101	82.896	12.845	27.780	1.00	31.52	C
	ATOM	5242	CD2	LEU	C	101	83.684	11.363	25.965	1.00	30.51	C
	ATOM	5243	C	LEU	C	101	82.067	15.347	24.904	1.00	34.53	C
	ATOM	5244	O	LEU	C	101	82.753	16.184	25.516	1.00	34.23	C
10	ATOM	5245	N	TYR	C	102	82.011	15.274	23.577	1.00	31.29	C
	ATOM	5246	CA	TYR	C	102	82.770	16.179	22.716	1.00	28.61	C
	ATOM	5247	CB	TYR	C	102	82.335	15.955	21.258	1.00	27.71	C
	ATOM	5248	CG	TYR	C	102	82.876	16.976	20.288	1.00	26.47	C
	ATOM	5249	CD1	TYR	C	102	84.220	16.970	19.896	1.00	24.67	C
15	ATOM	5250	CE1	TYR	C	102	84.708	17.930	19.005	1.00	23.69	C
	ATOM	5251	CD2	TYR	C	102	82.040	17.960	19.774	1.00	25.15	C
	ATOM	5252	CE2	TYR	C	102	82.505	18.913	18.899	1.00	23.80	C
	ATOM	5253	CZ	TYR	C	102	83.827	18.899	18.512	1.00	23.80	C
	ATOM	5254	OH	TYR	C	102	84.237	19.853	17.626	1.00	21.51	C
20	ATOM	5255	C	TYR	C	102	82.572	17.659	23.131	1.00	27.38	C
	ATOM	5256	O	TYR	C	102	83.536	18.383	23.433	1.00	23.78	C
	ATOM	5257	N	GLU	C	103	81.314	18.092	23.155	1.00	28.53	C
	ATOM	5258	CA	GLU	C	103	80.979	19.462	23.532	1.00	29.26	C
	ATOM	5259	CB	GLU	C	103	79.483	19.706	23.342	1.00	30.52	C
25	ATOM	5260	CG	GLU	C	103	79.063	19.574	21.888	1.00	33.75	C
	ATOM	5261	CD	GLU	C	103	77.781	20.318	21.565	1.00	36.95	C
	ATOM	5262	OE1	GLU	C	103	77.729	21.549	21.820	1.00	41.36	C
	ATOM	5263	OE2	GLU	C	103	76.832	19.682	21.053	1.00	35.81	C
	ATOM	5264	C	GLU	C	103	81.397	19.817	24.954	1.00	27.19	C
30	ATOM	5265	O	GLU	C	103	81.801	20.950	25.217	1.00	27.16	C
	ATOM	5266	N	ILE	C	104	81.317	18.855	25.870	1.00	26.37	C
	ATOM	5267	CA	ILE	C	104	81.717	19.114	27.254	1.00	25.70	C
	ATOM	5268	CB	ILE	C	104	81.356	17.913	28.167	1.00	25.25	C
	ATOM	5269	CG2	ILE	C	104	82.091	17.986	29.485	1.00	25.29	C
35	ATOM	5270	CG1	ILE	C	104	79.859	17.935	28.450	1.00	25.32	C
	ATOM	5271	CD1	ILE	C	104	79.346	16.709	29.127	1.00	25.12	C
	ATOM	5272	C	ILE	C	104	83.210	19.423	27.310	1.00	24.54	C
	ATOM	5273	O	ILE	C	104	83.614	20.452	27.848	1.00	22.76	C
	ATOM	5274	N	ILE	C	105	84.011	18.528	26.731	1.00	24.67	C
40	ATOM	5275	CA	ILE	C	105	85.464	18.687	26.673	1.00	23.37	C
	ATOM	5276	CB	ILE	C	105	86.120	17.563	25.834	1.00	22.40	C
	ATOM	5277	CG2	ILE	C	105	87.524	17.985	25.410	1.00	22.41	C
	ATOM	5278	CG1	ILE	C	105	86.143	16.249	26.630	1.00	22.74	C
	ATOM	5279	CD1	ILE	C	105	86.616	15.035	25.826	1.00	19.84	C
45	ATOM	5280	C	ILE	C	105	85.844	20.038	26.057	1.00	24.11	C
	ATOM	5281	O	ILE	C	105	86.885	20.601	26.383	1.00	23.21	C
	ATOM	5282	N	LEU	C	106	85.007	20.568	25.170	1.00	25.59	C
	ATOM	5283	CA	LEU	C	106	85.341	21.845	24.546	1.00	26.22	C
	ATOM	5284	CB	LEU	C	106	84.550	22.060	23.251	1.00	24.35	C
50	ATOM	5285	CG	LEU	C	106	84.955	21.288	21.982	1.00	24.05	C
	ATOM	5286	CD1	LEU	C	106	84.041	21.702	20.824	1.00	19.50	C
	ATOM	5287	CD2	LEU	C	106	86.411	21.582	21.631	1.00	19.81	C
	ATOM	5288	C	LEU	C	106	85.051	22.972	25.504	1.00	27.00	C
	ATOM	5289	O	LEU	C	106	85.876	23.871	25.700	1.00	28.04	C

	ATOM	5290	N	ALA	C	107	83.870	22.908	26.107	1.00	27.32	C
	ATOM	5291	CA	ALA	C	107	83.432	23.921	27.054	1.00	27.07	C
	ATOM	5292	CB	ALA	C	107	82.044	23.574	27.562	1.00	27.09	C
	ATOM	5293	C	ALA	C	107	84.417	23.967	28.210	1.00	26.97	C
5	ATOM	5294	O	ALA	C	107	84.759	25.040	28.720	1.00	25.71	C
	ATOM	5295	N	ALA	C	108	84.866	22.786	28.621	1.00	27.46	C
	ATOM	5296	CA	ALA	C	108	85.809	22.688	29.726	1.00	28.55	C
	ATOM	5297	CB	ALA	C	108	86.059	21.230	30.069	1.00	27.60	C
	ATOM	5298	C	ALA	C	108	87.119	23.383	29.363	1.00	29.01	C
10	ATOM	5299	O	ALA	C	108	87.595	24.264	30.085	1.00	29.74	C
	ATOM	5300	N	ASN	C	109	87.684	22.988	28.227	1.00	28.31	C
	ATOM	5301	CA	ASN	C	109	88.934	23.554	27.723	1.00	27.27	C
	ATOM	5302	CB	ASN	C	109	89.213	22.988	26.323	1.00	27.05	C
	ATOM	5303	CG	ASN	C	109	90.436	23.594	25.666	1.00	24.65	C
15	ATOM	5304	OD1	ASN	C	109	91.542	23.472	26.167	1.00	22.66	C
	ATOM	5305	ND2	ASN	C	109	90.236	24.235	24.517	1.00	24.60	C
	ATOM	5306	C	ASN	C	109	88.848	25.074	27.661	1.00	27.03	C
	ATOM	5307	O	ASN	C	109	89.755	25.770	28.109	1.00	28.21	C
	ATOM	5308	N	TYR	C	110	87.743	25.575	27.118	1.00	26.52	C
20	ATOM	5309	CA	TYR	C	110	87.528	27.003	26.969	1.00	26.57	C
	ATOM	5310	CB	TYR	C	110	86.268	27.267	26.139	1.00	25.48	C
	ATOM	5311	CG	TYR	C	110	85.938	28.734	26.018	1.00	24.82	C
	ATOM	5312	CD1	TYR	C	110	86.780	29.596	25.317	1.00	26.81	C
	ATOM	5313	CE1	TYR	C	110	86.543	30.968	25.273	1.00	26.16	C
25	ATOM	5314	CD2	TYR	C	110	84.838	29.282	26.669	1.00	24.41	C
	ATOM	5315	CE2	TYR	C	110	84.596	30.658	26.628	1.00	24.83	C
	ATOM	5316	CZ	TYR	C	110	85.455	31.486	25.930	1.00	24.87	C
	ATOM	5317	OH	TYR	C	110	85.234	32.835	25.889	1.00	25.53	C
	ATOM	5318	C	TYR	C	110	87.371	27.682	28.308	1.00	27.74	C
30	ATOM	5319	O	TYR	C	110	87.907	28.767	28.546	1.00	27.37	C
	ATOM	5320	N	LEU	C	111	86.610	27.040	29.178	1.00	28.23	C
	ATOM	5321	CA	LEU	C	111	86.348	27.593	30.485	1.00	28.18	C
	ATOM	5322	CB	LEU	C	111	85.067	26.958	31.031	1.00	25.97	C
	ATOM	5323	CG	LEU	C	111	83.874	27.827	31.434	1.00	24.04	C
35	ATOM	5324	CD1	LEU	C	111	83.755	29.132	30.657	1.00	19.70	C
	ATOM	5325	CD2	LEU	C	111	82.653	26.963	31.273	1.00	24.33	C
	ATOM	5326	C	LEU	C	111	87.547	27.373	31.410	1.00	29.42	C
	ATOM	5327	O	LEU	C	111	87.524	27.765	32.578	1.00	31.45	C
	ATOM	5328	N	ASN	C	112	88.601	26.761	30.875	1.00	29.81	C
40	ATOM	5329	CA	ASN	C	112	89.825	26.513	31.640	1.00	31.10	C
	ATOM	5330	CB	ASN	C	112	90.498	27.835	32.006	1.00	31.09	C
	ATOM	5331	CG	ASN	C	112	91.974	27.673	32.371	1.00	32.09	C
	ATOM	5332	OD1	ASN	C	112	92.448	26.579	32.719	1.00	29.20	C
	ATOM	5333	ND2	ASN	C	112	92.708	28.783	32.300	1.00	33.07	C
45	ATOM	5334	C	ASN	C	112	89.563	25.740	32.927	1.00	32.17	C
	ATOM	5335	O	ASN	C	112	89.805	26.237	34.030	1.00	33.29	C
	ATOM	5336	N	ILE	C	113	89.055	24.527	32.789	1.00	31.11	C
	ATOM	5337	CA	ILE	C	113	88.798	23.717	33.954	1.00	30.18	C
	ATOM	5338	CB	ILE	C	113	87.322	23.467	34.163	1.00	30.05	C
50	ATOM	5339	CG2	ILE	C	113	87.131	22.660	35.442	1.00	28.92	C
	ATOM	5340	CG1	ILE	C	113	86.564	24.789	34.234	1.00	28.96	C
	ATOM	5341	CD1	ILE	C	113	85.076	24.575	34.283	1.00	28.52	C
	ATOM	5342	C	ILE	C	113	89.473	22.384	33.751	1.00	30.85	C
	ATOM	5343	O	ILE	C	113	88.834	21.400	33.387	1.00	29.72	C

	ATOM	5344	N	LYS	C	114	90.778	22.368	33.998	1.00	31.38	C
	ATOM	5345	CA	LYS	C	114	91.595	21.173	33.838	1.00	31.36	C
	ATOM	5346	CB	LYS	C	114	93.003	21.440	34.383	1.00	32.37	C
	ATOM	5347	CG	LYS	C	114	93.901	20.219	34.344	1.00	34.25	C
5	ATOM	5348	CD	LYS	C	114	95.372	20.555	34.550	1.00	35.39	C
	ATOM	5349	CE	LYS	C	114	96.190	19.289	34.455	1.00	36.88	C
	ATOM	5350	NZ	LYS	C	114	95.863	18.587	33.190	1.00	40.06	C
	ATOM	5351	C	LYS	C	114	91.035	19.876	34.437	1.00	30.61	C
	ATOM	5352	O	LYS	C	114	91.054	18.841	33.785	1.00	30.70	C
10	ATOM	5353	N	PRO	C	115	90.530	19.916	35.681	1.00	30.70	C
	ATOM	5354	CD	PRO	C	115	90.401	21.106	36.545	1.00	31.09	C
	ATOM	5355	CA	PRO	C	115	89.970	18.719	36.338	1.00	30.04	C
	ATOM	5356	CB	PRO	C	115	89.365	19.276	37.626	1.00	30.45	C
	ATOM	5357	CG	PRO	C	115	90.220	20.489	37.912	1.00	31.85	C
15	ATOM	5358	C	PRO	C	115	88.914	18.030	35.482	1.00	29.80	C
	ATOM	5359	O	PRO	C	115	88.935	16.806	35.295	1.00	30.05	C
	ATOM	5360	N	LEU	C	116	87.981	18.833	34.974	1.00	29.91	C
	ATOM	5361	CA	LEU	C	116	86.904	18.330	34.114	1.00	29.38	C
	ATOM	5362	CB	LEU	C	116	85.797	19.376	33.980	1.00	27.77	C
20	ATOM	5363	CG	LEU	C	116	84.628	18.909	33.138	1.00	27.38	C
	ATOM	5364	CD1	LEU	C	116	84.043	17.676	33.768	1.00	27.48	C
	ATOM	5365	CD2	LEU	C	116	83.597	20.023	33.027	1.00	27.97	C
	ATOM	5366	C	LEU	C	116	87.464	17.974	32.731	1.00	28.24	C
	ATOM	5367	O	LEU	C	116	87.042	17.003	32.107	1.00	28.34	C
25	ATOM	5368	N	LEU	C	117	88.433	18.756	32.272	1.00	26.39	C
	ATOM	5369	CA	LEU	C	117	89.051	18.494	30.993	1.00	26.69	C
	ATOM	5370	CB	LEU	C	117	90.112	19.547	30.701	1.00	24.99	C
	ATOM	5371	CG	LEU	C	117	90.893	19.362	29.397	1.00	24.42	C
	ATOM	5372	CD1	LEU	C	117	89.943	19.112	28.225	1.00	23.60	C
30	ATOM	5373	CD2	LEU	C	117	91.738	20.593	29.154	1.00	22.70	C
	ATOM	5374	C	LEU	C	117	89.680	17.100	30.981	1.00	28.34	C
	ATOM	5375	O	LEU	C	117	89.397	16.288	30.093	1.00	29.22	C
	ATOM	5376	N	ASP	C	118	90.528	16.826	31.973	1.00	29.30	C
	ATOM	5377	CA	ASP	C	118	91.207	15.532	32.105	1.00	29.52	C
35	ATOM	5378	CB	ASP	C	118	92.117	15.538	33.347	1.00	32.96	C
	ATOM	5379	CG	ASP	C	118	93.158	16.668	33.316	1.00	36.46	C
	ATOM	5380	OD1	ASP	C	118	93.138	17.470	32.353	1.00	37.36	C
	ATOM	5381	OD2	ASP	C	118	93.990	16.757	34.253	1.00	36.80	C
	ATOM	5382	C	ASP	C	118	90.213	14.365	32.186	1.00	28.84	C
40	ATOM	5383	O	ASP	C	118	90.289	13.418	31.391	1.00	28.39	C
	ATOM	5384	N	ALA	C	119	89.288	14.419	33.142	1.00	26.34	C
	ATOM	5385	CA	ALA	C	119	88.293	13.348	33.262	1.00	25.58	C
	ATOM	5386	CB	ALA	C	119	87.208	13.741	34.258	1.00	26.08	C
	ATOM	5387	C	ALA	C	119	87.654	13.022	31.899	1.00	24.81	C
45	ATOM	5388	O	ALA	C	119	87.489	11.852	31.540	1.00	23.57	C
	ATOM	5389	N	GLY	C	120	87.282	14.060	31.154	1.00	22.99	C
	ATOM	5390	CA	GLY	C	120	86.695	13.840	29.850	1.00	23.36	C
	ATOM	5391	C	GLY	C	120	87.654	13.095	28.932	1.00	23.32	C
	ATOM	5392	O	GLY	C	120	87.284	12.124	28.282	1.00	22.39	C
50	ATOM	5393	N	CYS	C	121	88.902	13.541	28.901	1.00	23.17	C
	ATOM	5394	CA	CYS	C	121	89.918	12.935	28.065	1.00	23.66	C
	ATOM	5395	CB	CYS	C	121	91.184	13.762	28.144	1.00	24.22	C
	ATOM	5396	SG	CYS	C	121	90.981	15.370	27.390	1.00	31.59	C
	ATOM	5397	C	CYS	C	121	90.215	11.497	28.425	1.00	24.08	C

	ATOM	5398	O	CYS	C	121	90.601	10.703	27.570	1.00	25.40	C
	ATOM	5399	N	LYS	C	122	90.026	11.155	29.692	1.00	25.04	C
	ATOM	5400	CA	LYS	C	122	90.270	9.796	30.138	1.00	24.59	C
	ATOM	5401	CB	LYS	C	122	90.293	9.740	31.672	1.00	25.68	C
5	ATOM	5402	CG	LYS	C	122	91.396	10.599	32.270	1.00	26.14	C
	ATOM	5403	CD	LYS	C	122	91.580	10.400	33.763	1.00	27.91	C
	ATOM	5404	CE	LYS	C	122	92.594	11.421	34.315	1.00	29.43	C
	ATOM	5405	NZ	LYS	C	122	93.121	11.095	35.679	1.00	31.16	C
	ATOM	5406	C	LYS	C	122	89.179	8.897	29.571	1.00	24.85	C
10	ATOM	5407	O	LYS	C	122	89.451	7.798	29.080	1.00	24.38	C
	ATOM	5408	N	VAL	C	123	87.940	9.366	29.611	1.00	26.05	C
	ATOM	5409	CA	VAL	C	123	86.856	8.555	29.071	1.00	27.70	C
	ATOM	5410	CB	VAL	C	123	85.509	9.274	29.197	1.00	28.31	C
	ATOM	5411	CG1	VAL	C	123	84.389	8.383	28.667	1.00	28.23	C
15	ATOM	5412	CG2	VAL	C	123	85.272	9.627	30.650	1.00	26.87	C
	ATOM	5413	C	VAL	C	123	87.142	8.223	27.606	1.00	27.72	C
	ATOM	5414	O	VAL	C	123	86.946	7.083	27.165	1.00	27.83	C
	ATOM	5415	N	VAL	C	124	87.618	9.212	26.855	1.00	27.26	C
	ATOM	5416	CA	VAL	C	124	87.947	8.982	25.452	1.00	27.88	C
20	ATOM	5417	CB	VAL	C	124	88.458	10.274	24.776	1.00	26.84	C
	ATOM	5418	CG1	VAL	C	124	88.953	9.959	23.368	1.00	26.47	C
	ATOM	5419	CG2	VAL	C	124	87.322	11.304	24.713	1.00	23.58	C
	ATOM	5420	C	VAL	C	124	89.008	7.880	25.343	1.00	28.21	C
	ATOM	5421	O	VAL	C	124	88.830	6.898	24.599	1.00	27.09	C
25	ATOM	5422	N	ALA	C	125	90.097	8.041	26.095	1.00	26.95	C
	ATOM	5423	CA	ALA	C	125	91.170	7.050	26.102	1.00	29.33	C
	ATOM	5424	CB	ALA	C	125	92.268	7.479	27.044	1.00	27.76	C
	ATOM	5425	C	ALA	C	125	90.653	5.661	26.501	1.00	31.95	C
	ATOM	5426	O	ALA	C	125	91.063	4.647	25.930	1.00	32.25	C
30	ATOM	5427	N	GLU	C	126	89.749	5.617	27.476	1.00	34.71	C
	ATOM	5428	CA	GLU	C	126	89.179	4.356	27.919	1.00	36.70	C
	ATOM	5429	CB	GLU	C	126	88.333	4.572	29.173	1.00	39.48	C
	ATOM	5430	CG	GLU	C	126	87.803	3.290	29.782	1.00	45.29	C
	ATOM	5431	CD	GLU	C	126	88.919	2.320	30.166	1.00	50.81	C
35	ATOM	5432	OE1	GLU	C	126	89.934	2.813	30.740	1.00	52.04	C
	ATOM	5433	OE2	GLU	C	126	88.780	1.083	29.904	1.00	50.45	C
	ATOM	5434	C	GLU	C	126	88.325	3.739	26.813	1.00	35.98	C
	ATOM	5435	O	GLU	C	126	87.849	2.628	26.968	1.00	33.64	C
	ATOM	5436	N	MSE	C	127	88.123	4.477	25.717	1.00	37.74	C
40	ATOM	5437	CA	MSE	C	127	87.355	3.994	24.563	1.00	39.73	C
	ATOM	5438	CB	MSE	C	127	86.592	5.129	23.866	1.00	41.63	C
	ATOM	5439	CG	MSE	C	127	85.526	5.848	24.700	1.00	42.19	C
	ATOM	5440	SE	MSE	C	127	84.412	7.110	23.629	1.00	43.57	C
	ATOM	5441	CE	MSE	C	127	82.969	5.916	23.133	1.00	43.96	C
45	ATOM	5442	C	MSE	C	127	88.295	3.377	23.530	1.00	40.34	C
	ATOM	5443	O	MSE	C	127	87.885	2.517	22.753	1.00	41.30	C
	ATOM	5444	N	ILE	C	128	89.544	3.835	23.506	1.00	40.42	C
	ATOM	5445	CA	ILE	C	128	90.516	3.309	22.559	1.00	39.85	C
	ATOM	5446	CB	ILE	C	128	91.552	4.378	22.130	1.00	39.70	C
50	ATOM	5447	CG2	ILE	C	128	92.689	3.746	21.349	1.00	39.51	C
	ATOM	5448	CG1	ILE	C	128	90.879	5.426	21.254	1.00	38.45	C
	ATOM	5449	CD1	ILE	C	128	90.118	6.401	22.035	1.00	40.80	C
	ATOM	5450	C	ILE	C	128	91.245	2.174	23.224	1.00	39.58	C
	ATOM	5451	O	ILE	C	128	91.534	1.156	22.603	1.00	40.22	C

	ATOM	5452	N	ARG	C	129	91.518	2.353	24.508	1.00	39.78	C
	ATOM	5453	CA	ARG	C	129	92.230	1.362	25.300	1.00	38.47	C
	ATOM	5454	CB	ARG	C	129	91.959	1.599	26.781	1.00	39.40	C
	ATOM	5455	CG	ARG	C	129	93.052	1.083	27.689	1.00	38.81	C
5	ATOM	5456	CD	ARG	C	129	92.731	1.379	29.130	1.00	40.09	C
	ATOM	5457	NE	ARG	C	129	92.640	2.812	29.456	1.00	42.40	C
	ATOM	5458	CZ	ARG	C	129	93.651	3.680	29.437	1.00	41.54	C
	ATOM	5459	NH1	ARG	C	129	94.869	3.283	29.089	1.00	41.83	C
	ATOM	5460	NH2	ARG	C	129	93.443	4.937	29.815	1.00	39.32	C
10	ATOM	5461	C	ARG	C	129	91.863	-0.066	24.940	1.00	37.14	C
	ATOM	5462	O	ARG	C	129	90.682	-0.428	24.875	1.00	34.49	C
	ATOM	5463	N	GLY	C	130	92.900	-0.860	24.688	1.00	36.58	C
	ATOM	5464	CA	GLY	C	130	92.732	-2.264	24.356	1.00	36.84	C
	ATOM	5465	C	GLY	C	130	92.098	-2.656	23.032	1.00	36.85	C
15	ATOM	5466	O	GLY	C	130	92.210	-3.816	22.626	1.00	37.50	C
	ATOM	5467	N	ARG	C	131	91.431	-1.721	22.359	1.00	37.11	C
	ATOM	5468	CA	ARG	C	131	90.787	-2.017	21.073	1.00	37.10	C
	ATOM	5469	CB	ARG	C	131	89.711	-0.973	20.771	1.00	39.22	C
	ATOM	5470	CG	ARG	C	131	88.431	-1.131	21.569	1.00	41.84	C
20	ATOM	5471	CD	ARG	C	131	87.839	-2.509	21.363	1.00	45.09	C
	ATOM	5472	NE	ARG	C	131	86.396	-2.558	21.604	1.00	47.90	C
	ATOM	5473	CZ	ARG	C	131	85.479	-2.055	20.780	1.00	49.21	C
	ATOM	5474	NH1	ARG	C	131	85.846	-1.459	19.656	1.00	49.53	C
	ATOM	5475	NH2	ARG	C	131	84.191	-2.155	21.073	1.00	51.64	C
25	ATOM	5476	C	ARG	C	131	91.760	-2.084	19.894	1.00	35.38	C
	ATOM	5477	O	ARG	C	131	92.917	-1.676	19.989	1.00	34.16	C
	ATOM	5478	N	SER	C	132	91.277	-2.610	18.781	1.00	33.40	C
	ATOM	5479	CA	SER	C	132	92.093	-2.717	17.585	1.00	32.90	C
	ATOM	5480	CB	SER	C	132	91.933	-4.096	16.966	1.00	31.03	C
30	ATOM	5481	OG	SER	C	132	90.581	-4.307	16.607	1.00	31.69	C
	ATOM	5482	C	SER	C	132	91.646	-1.661	16.576	1.00	32.11	C
	ATOM	5483	O	SER	C	132	90.585	-1.054	16.738	1.00	30.91	C
	ATOM	5484	N	PRO	C	133	92.462	-1.422	15.532	1.00	31.16	C
	ATOM	5485	CD	PRO	C	133	93.848	-1.900	15.407	1.00	29.35	C
35	ATOM	5486	CA	PRO	C	133	92.180	-0.451	14.480	1.00	32.65	C
	ATOM	5487	CB	PRO	C	133	93.219	-0.801	13.441	1.00	29.52	C
	ATOM	5488	CG	PRO	C	133	94.400	-1.021	14.307	1.00	29.23	C
	ATOM	5489	C	PRO	C	133	90.754	-0.514	13.963	1.00	35.83	C
	ATOM	5490	O	PRO	C	133	90.054	0.504	13.909	1.00	36.35	C
40	ATOM	5491	N	GLU	C	134	90.318	-1.709	13.588	1.00	38.45	C
	ATOM	5492	CA	GLU	C	134	88.962	-1.875	13.104	1.00	41.11	C
	ATOM	5493	CB	GLU	C	134	88.765	-3.265	12.494	1.00	44.05	C
	ATOM	5494	CG	GLU	C	134	88.697	-3.264	10.965	1.00	49.94	C
	ATOM	5495	CD	GLU	C	134	87.779	-2.177	10.405	1.00	52.39	C
45	ATOM	5496	OE1	GLU	C	134	86.664	-2.011	10.958	1.00	54.43	C
	ATOM	5497	OE2	GLU	C	134	88.173	-1.503	9.413	1.00	51.18	C
	ATOM	5498	C	GLU	C	134	87.968	-1.660	14.249	1.00	41.19	C
	ATOM	5499	O	GLU	C	134	86.913	-1.040	14.062	1.00	40.64	C
50	ATOM	5500	N	GLU	C	135	88.297	-2.162	15.437	1.00	41.33	C
	ATOM	5501	CA	GLU	C	135	87.399	-1.978	16.575	1.00	42.01	C
	ATOM	5502	CB	GLU	C	135	87.915	-2.697	17.820	1.00	42.98	C
	ATOM	5503	CG	GLU	C	135	87.961	-4.198	17.745	1.00	44.16	C
	ATOM	5504	CD	GLU	C	135	88.393	-4.796	19.073	1.00	46.95	C
	ATOM	5505	OE1	GLU	C	135	89.419	-4.323	19.629	1.00	46.77	C

	ATOM	5506	OE2	GLU	C	135	87.712	-5.728	19.565	1.00	48.28	C
	ATOM	5507	C	GLU	C	135	87.226	-0.489	16.908	1.00	40.82	C
	ATOM	5508	O	GLU	C	135	86.152	-0.055	17.328	1.00	42.69	C
	ATOM	5509	N	ILE	C	136	88.284	0.292	16.718	1.00	37.69	C
5	ATOM	5510	CA	ILE	C	136	88.224	1.718	16.997	1.00	33.59	C
	ATOM	5511	CB	ILE	C	136	89.638	2.316	17.096	1.00	32.05	C
	ATOM	5512	CG2	ILE	C	136	89.552	3.838	17.349	1.00	27.02	C
	ATOM	5513	CG1	ILE	C	136	90.412	1.564	18.196	1.00	29.01	C
	ATOM	5514	CD1	ILE	C	136	91.859	1.992	18.390	1.00	26.23	C
10	ATOM	5515	C	ILE	C	136	87.442	2.419	15.903	1.00	33.18	C
	ATOM	5516	O	ILE	C	136	86.631	3.299	16.171	1.00	31.83	C
	ATOM	5517	N	ARG	C	137	87.669	2.021	14.661	1.00	34.42	C
	ATOM	5518	CA	ARG	C	137	86.955	2.652	13.566	1.00	34.64	C
	ATOM	5519	CB	ARG	C	137	87.352	2.008	12.253	1.00	33.73	C
15	ATOM	5520	CG	ARG	C	137	88.809	2.218	11.916	1.00	34.55	C
	ATOM	5521	CD	ARG	C	137	89.226	1.238	10.851	1.00	34.62	C
	ATOM	5522	NE	ARG	C	137	90.665	1.216	10.644	1.00	33.99	C
	ATOM	5523	CZ	ARG	C	137	91.340	0.120	10.328	1.00	34.12	C
	ATOM	5524	NH1	ARG	C	137	90.694	-1.029	10.197	1.00	32.84	C
20	ATOM	5525	NH2	ARG	C	137	92.651	0.176	10.125	1.00	34.77	C
	ATOM	5526	C	ARG	C	137	85.454	2.549	13.774	1.00	35.03	C
	ATOM	5527	O	ARG	C	137	84.745	3.538	13.638	1.00	34.65	C
	ATOM	5528	N	ARG	C	138	84.968	1.366	14.132	1.00	35.13	C
	ATOM	5529	CA	ARG	C	138	83.539	1.211	14.328	1.00	36.00	C
25	ATOM	5530	CB	ARG	C	138	83.176	-0.270	14.439	1.00	38.78	C
	ATOM	5531	CG	ARG	C	138	83.339	-1.037	13.114	1.00	43.46	C
	ATOM	5532	CD	ARG	C	138	82.329	-0.608	12.030	0.00	47.14	C
	ATOM	5533	NE	ARG	C	138	82.537	0.734	11.466	0.00	51.00	C
	ATOM	5534	CZ	ARG	C	138	83.462	1.061	10.563	1.00	54.05	C
30	ATOM	5535	NH1	ARG	C	138	84.302	0.146	10.095	1.00	55.91	C
	ATOM	5536	NH2	ARG	C	138	83.532	2.307	10.105	1.00	54.20	C
	ATOM	5537	C	ARG	C	138	83.008	1.990	15.528	1.00	34.39	C
	ATOM	5538	O	ARG	C	138	81.816	2.264	15.626	1.00	34.40	C
	ATOM	5539	N	THR	C	139	83.895	2.377	16.426	1.00	31.97	C
35	ATOM	5540	CA	THR	C	139	83.486	3.123	17.596	1.00	29.98	C
	ATOM	5541	CB	THR	C	139	84.575	3.077	18.624	1.00	30.24	C
	ATOM	5542	OG1	THR	C	139	84.946	1.713	18.825	1.00	31.86	C
	ATOM	5543	CG2	THR	C	139	84.120	3.697	19.923	1.00	28.26	C
	ATOM	5544	C	THR	C	139	83.214	4.573	17.265	1.00	29.86	C
40	ATOM	5545	O	THR	C	139	82.267	5.180	17.767	1.00	30.37	C
	ATOM	5546	N	PHE	C	140	84.053	5.138	16.415	1.00	29.19	C
	ATOM	5547	CA	PHE	C	140	83.883	6.525	16.045	1.00	28.27	C
	ATOM	5548	CB	PHE	C	140	85.229	7.230	16.152	1.00	25.82	C
	ATOM	5549	CG	PHE	C	140	85.797	7.223	17.537	1.00	23.52	C
45	ATOM	5550	CD1	PHE	C	140	85.228	7.990	18.543	1.00	22.27	C
	ATOM	5551	CD2	PHE	C	140	86.907	6.452	17.844	1.00	22.34	C
	ATOM	5552	CE1	PHE	C	140	85.767	7.982	19.839	1.00	20.23	C
	ATOM	5553	CE2	PHE	C	140	87.450	6.441	19.135	1.00	18.70	C
	ATOM	5554	CZ	PHE	C	140	86.880	7.204	20.126	1.00	17.04	C
50	ATOM	5555	C	PHE	C	140	83.307	6.697	14.647	1.00	28.75	C
	ATOM	5556	O	PHE	C	140	83.087	7.822	14.221	1.00	30.09	C
	ATOM	5557	N	ASN	C	141	83.027	5.585	13.964	1.00	29.40	C
	ATOM	5558	CA	ASN	C	141	82.521	5.589	12.580	1.00	30.10	C
	ATOM	5559	CB	ASN	C	141	81.182	6.335	12.434	1.00	30.86	C

	ATOM	5560	CG	ASN	C	141	80.620	6.279	10.991	1.00	32.35	C
	ATOM	5561	OD1	ASN	C	141	80.549	5.206	10.385	1.00	30.84	C
	ATOM	5562	ND2	ASN	C	141	80.212	7.436	10.453	1.00	32.26	C
	ATOM	5563	C	ASN	C	141	83.554	6.256	11.680	1.00	30.32	C
5	ATOM	5564	O	ASN	C	141	83.223	7.047	10.803	1.00	31.59	C
	ATOM	5565	N	ILE	C	142	84.821	5.953	11.907	1.00	29.73	C
	ATOM	5566	CA	ILE	C	142	85.867	6.548	11.091	1.00	30.11	C
	ATOM	5567	CB	ILE	C	142	87.151	6.830	11.983	1.00	29.75	C
	ATOM	5568	CG2	ILE	C	142	87.180	5.925	13.180	1.00	31.60	C
10	ATOM	5569	CG1	ILE	C	142	88.428	6.712	11.164	1.00	29.84	C
	ATOM	5570	CD1	ILE	C	142	88.925	8.056	10.663	1.00	36.02	C
	ATOM	5571	C	ILE	C	142	86.129	5.630	9.885	1.00	28.78	C
	ATOM	5572	O	ILE	C	142	86.070	4.412	10.004	1.00	27.70	C
	ATOM	5573	N	VAL	C	143	86.355	6.201	8.708	1.00	28.81	C
15	ATOM	5574	CA	VAL	C	143	86.594	5.344	7.556	1.00	28.92	C
	ATOM	5575	CB	VAL	C	143	86.022	5.937	6.250	1.00	27.33	C
	ATOM	5576	CG1	VAL	C	143	86.549	5.165	5.056	1.00	27.92	C
	ATOM	5577	CG2	VAL	C	143	84.494	5.866	6.269	1.00	26.26	C
	ATOM	5578	C	VAL	C	143	88.071	5.084	7.356	1.00	28.95	C
20	ATOM	5579	O	VAL	C	143	88.905	5.971	7.539	1.00	31.52	C
	ATOM	5580	N	ASN	C	144	88.387	3.845	7.006	1.00	27.50	C
	ATOM	5581	CA	ASN	C	144	89.754	3.434	6.761	1.00	26.06	C
	ATOM	5582	CB	ASN	C	144	89.837	1.907	6.798	1.00	27.42	C
	ATOM	5583	CG	ASN	C	144	91.258	1.377	6.661	1.00	28.39	C
25	ATOM	5584	OD1	ASN	C	144	91.528	0.242	7.035	1.00	28.70	C
	ATOM	5585	ND2	ASN	C	144	92.162	2.185	6.119	1.00	30.75	C
	ATOM	5586	C	ASN	C	144	90.074	3.942	5.371	1.00	26.48	C
	ATOM	5587	O	ASN	C	144	89.519	3.458	4.394	1.00	26.51	C
	ATOM	5588	N	ASP	C	145	90.964	4.918	5.277	1.00	26.34	C
30	ATOM	5589	CA	ASP	C	145	91.315	5.492	3.988	1.00	27.61	C
	ATOM	5590	CB	ASP	C	145	91.245	7.018	4.058	1.00	28.15	C
	ATOM	5591	CG	ASP	C	145	91.840	7.570	5.336	1.00	28.20	C
	ATOM	5592	OD1	ASP	C	145	92.508	6.808	6.080	1.00	26.63	C
	ATOM	5593	OD2	ASP	C	145	91.639	8.780	5.595	1.00	29.52	C
35	ATOM	5594	C	ASP	C	145	92.684	5.086	3.479	1.00	28.92	C
	ATOM	5595	O	ASP	C	145	93.208	5.708	2.549	1.00	29.06	C
	ATOM	5596	N	PHE	C	146	93.262	4.050	4.083	1.00	28.68	C
	ATOM	5597	CA	PHE	C	146	94.585	3.572	3.685	1.00	29.48	C
	ATOM	5598	CB	PHE	C	146	95.222	2.744	4.799	1.00	31.05	C
40	ATOM	5599	CG	PHE	C	146	95.709	3.550	5.955	1.00	33.63	C
	ATOM	5600	CD1	PHE	C	146	96.641	4.574	5.761	1.00	34.53	C
	ATOM	5601	CD2	PHE	C	146	95.277	3.254	7.250	1.00	33.58	C
	ATOM	5602	CE1	PHE	C	146	97.147	5.292	6.841	1.00	35.14	C
	ATOM	5603	CE2	PHE	C	146	95.767	3.956	8.338	1.00	34.74	C
45	ATOM	5604	CZ	PHE	C	146	96.709	4.981	8.136	1.00	36.19	C
	ATOM	5605	C	PHE	C	146	94.596	2.727	2.431	1.00	28.86	C
	ATOM	5606	O	PHE	C	146	93.889	1.725	2.355	1.00	30.57	C
	ATOM	5607	N	THR	C	147	95.423	3.109	1.460	1.00	28.83	C
	ATOM	5608	CA	THR	C	147	95.536	2.339	0.222	1.00	30.01	C
50	ATOM	5609	CB	THR	C	147	96.556	2.946	-0.783	1.00	29.36	C
	ATOM	5610	OG1	THR	C	147	97.817	3.147	-0.128	1.00	29.97	C
	ATOM	5611	CG2	THR	C	147	96.046	4.252	-1.355	1.00	27.00	C
	ATOM	5612	C	THR	C	147	96.049	0.948	0.552	1.00	30.37	C
	ATOM	5613	O	THR	C	147	96.708	0.745	1.563	1.00	31.13	C

	ATOM	5614	N	PRO	C	148	95.751	-0.032	-0.299	1.00	31.61	C
	ATOM	5615	CD	PRO	C	148	94.879	-0.031	-1.485	1.00	31.67	C
	ATOM	5616	CA	PRO	C	148	96.241	-1.375	-0.010	1.00	32.60	C
	ATOM	5617	CB	PRO	C	148	95.903	-2.141	-1.282	1.00	31.26	C
5	ATOM	5618	CG	PRO	C	148	94.611	-1.527	-1.697	1.00	30.19	C
	ATOM	5619	C	PRO	C	148	97.734	-1.327	0.255	1.00	34.28	C
	ATOM	5620	O	PRO	C	148	98.244	-2.067	1.087	1.00	35.43	C
	ATOM	5621	N	GLU	C	149	98.441	-0.445	-0.437	1.00	37.73	C
	ATOM	5622	CA	GLU	C	149	99.873	-0.372	-0.221	1.00	41.17	C
10	ATOM	5623	CB	GLU	C	149	100.532	0.535	-1.266	1.00	39.75	C
	ATOM	5624	CG	GLU	C	149	102.038	0.662	-1.083	1.00	39.00	C
	ATOM	5625	CD	GLU	C	149	102.703	1.461	-2.171	1.00	39.73	C
	ATOM	5626	OE1	GLU	C	149	102.443	2.683	-2.265	1.00	39.67	C
	ATOM	5627	OE2	GLU	C	149	103.490	0.868	-2.938	1.00	39.04	C
15	ATOM	5628	C	GLU	C	149	100.183	0.120	1.195	1.00	44.52	C
	ATOM	5629	O	GLU	C	149	100.646	-0.656	2.032	1.00	44.69	C
	ATOM	5630	N	GLU	C	150	99.914	1.398	1.460	1.00	48.03	C
	ATOM	5631	CA	GLU	C	150	100.161	1.995	2.774	1.00	51.71	C
	ATOM	5632	CB	GLU	C	150	99.557	3.407	2.822	1.00	52.60	C
20	ATOM	5633	CG	GLU	C	150	100.095	4.362	1.763	1.00	56.26	C
	ATOM	5634	CD	GLU	C	150	101.508	4.869	2.052	1.00	57.57	C
	ATOM	5635	OE1	GLU	C	150	101.735	5.354	3.178	1.00	58.02	C
	ATOM	5636	OE2	GLU	C	150	102.381	4.803	1.153	1.00	58.12	C
	ATOM	5637	C	GLU	C	150	99.603	1.136	3.938	1.00	53.38	C
25	ATOM	5638	O	GLU	C	150	100.159	1.112	5.042	1.00	52.61	C
	ATOM	5639	N	GLU	C	151	98.515	0.420	3.677	1.00	55.17	C
	ATOM	5640	CA	GLU	C	151	97.891	-0.431	4.681	1.00	58.21	C
	ATOM	5641	CB	GLU	C	151	96.636	-1.087	4.097	1.00	60.47	C
	ATOM	5642	CG	GLU	C	151	95.349	-0.835	4.868	1.00	62.11	C
30	ATOM	5643	CD	GLU	C	151	94.154	-1.512	4.222	1.00	63.63	C
	ATOM	5644	OE1	GLU	C	151	94.025	-1.410	2.978	1.00	64.05	C
	ATOM	5645	OE2	GLU	C	151	93.347	-2.135	4.955	1.00	63.74	C
	ATOM	5646	C	GLU	C	151	98.845	-1.519	5.182	1.00	59.56	C
	ATOM	5647	O	GLU	C	151	99.118	-1.609	6.375	1.00	60.86	C
35	ATOM	5648	N	ALA	C	152	99.345	-2.346	4.269	1.00	60.60	C
	ATOM	5649	CA	ALA	C	152	100.263	-3.422	4.626	1.00	61.88	C
	ATOM	5650	CB	ALA	C	152	100.455	-4.356	3.439	1.00	61.89	C
	ATOM	5651	C	ALA	C	152	101.616	-2.881	5.080	1.00	62.64	C
	ATOM	5652	O	ALA	C	152	102.398	-3.589	5.699	1.00	62.91	C
40	ATOM	5653	N	ALA	C	153	101.888	-1.622	4.769	1.00	64.35	C
	ATOM	5654	CA	ALA	C	153	103.146	-1.005	5.144	1.00	66.65	C
	ATOM	5655	CB	ALA	C	153	103.441	0.166	4.222	1.00	66.57	C
	ATOM	5656	C	ALA	C	153	103.114	-0.534	6.593	1.00	68.35	C
	ATOM	5657	O	ALA	C	153	104.159	-0.238	7.177	1.00	67.40	C
45	ATOM	5658	N	ILE	C	154	101.913	-0.463	7.167	1.00	70.84	C
	ATOM	5659	CA	ILE	C	154	101.753	-0.021	8.549	1.00	73.04	C
	ATOM	5660	CB	ILE	C	154	100.276	0.333	8.874	1.00	72.44	C
	ATOM	5661	CG2	ILE	C	154	100.160	0.823	10.308	0.00	73.15	C
	ATOM	5662	CG1	ILE	C	154	99.768	1.405	7.906	0.00	73.18	C
50	ATOM	5663	CD1	ILE	C	154	100.596	2.681	7.891	0.00	73.32	C
	ATOM	5664	C	ILE	C	154	102.242	-1.083	9.530	1.00	74.39	C
	ATOM	5665	O	ILE	C	154	103.164	-0.836	10.314	1.00	75.10	C
	ATOM	5666	N	ARG	C	155	101.638	-2.267	9.481	1.00	75.33	C
	ATOM	5667	CA	ARG	C	155	102.035	-3.343	10.386	1.00	77.14	C

	ATOM	5668	CB	ARG	C	155	101.354	-4.655	9.970	1.00	77.56	C
	ATOM	5669	CG	ARG	C	155	101.473	-4.969	8.491	1.00	79.06	C
	ATOM	5670	CD	ARG	C	155	100.453	-6.012	8.042	1.00	79.84	C
	ATOM	5671	NE	ARG	C	155	101.032	-7.346	7.880	1.00	82.03	C
5	ATOM	5672	CZ	ARG	C	155	101.458	-8.120	8.876	1.00	83.21	C
	ATOM	5673	NH1	ARG	C	155	101.376	-7.702	10.130	1.00	83.46	C
	ATOM	5674	NH2	ARG	C	155	101.967	-9.320	8.617	1.00	83.34	C
	ATOM	5675	C	ARG	C	155	103.557	-3.521	10.429	1.00	77.49	C
	ATOM	5676	O	ARG	C	155	104.141	-3.689	11.505	1.00	76.81	C
10	ATOM	5677	N	ARG	C	156	104.185	-3.454	9.256	1.00	78.72	C
	ATOM	5678	CA	ARG	C	156	105.631	-3.611	9.120	1.00	80.26	C
	ATOM	5679	CB	ARG	C	156	106.371	-2.543	9.936	1.00	79.66	C
	ATOM	5680	CG	ARG	C	156	106.197	-1.128	9.442	1.00	78.84	C
	ATOM	5681	CD	ARG	C	156	106.951	-0.151	10.332	1.00	78.63	C
15	ATOM	5682	NE	ARG	C	156	106.958	1.201	9.777	1.00	79.37	C
	ATOM	5683	CZ	ARG	C	156	107.560	2.243	10.344	1.00	79.78	C
	ATOM	5684	NH1	ARG	C	156	108.210	2.098	11.492	1.00	80.21	C
	ATOM	5685	NH2	ARG	C	156	107.513	3.434	9.763	1.00	79.89	C
	ATOM	5686	C	ARG	C	156	106.075	-4.997	9.586	1.00	81.59	C
20	ATOM	5687	O	ARG	C	156	106.298	-5.862	8.715	0.00	81.82	C
	ATOM	5688	OXT	ARG	C	156	106.182	-5.207	10.817	1.00	83.28	C
	ATOM	5689	CB	LEU	D	270	75.377	10.305	15.206	1.00	63.79	D
	ATOM	5690	CG	LEU	D	270	75.038	9.447	13.983	1.00	64.88	D
	ATOM	5691	CD1	LEU	D	270	73.550	9.589	13.707	1.00	64.89	D
25	ATOM	5692	CD2	LEU	D	270	75.842	9.894	12.762	1.00	64.87	D
	ATOM	5693	C	LEU	D	270	77.526	9.458	16.216	1.00	61.89	D
	ATOM	5694	O	LEU	D	270	78.274	9.273	17.176	1.00	61.69	D
	ATOM	5695	N	LEU	D	270	75.776	10.456	17.643	1.00	62.12	D
	ATOM	5696	CA	LEU	D	270	76.015	9.627	16.425	1.00	62.72	D
30	ATOM	5697	N	LYS	D	271	77.975	9.523	14.966	1.00	60.94	D
	ATOM	5698	CA	LYS	D	271	79.394	9.377	14.666	1.00	59.23	D
	ATOM	5699	CB	LYS	D	271	79.635	9.177	13.157	1.00	61.06	D
	ATOM	5700	CG	LYS	D	271	79.243	10.362	12.273	1.00	61.84	D
	ATOM	5701	CD	LYS	D	271	79.810	10.233	10.859	1.00	62.36	D
35	ATOM	5702	CE	LYS	D	271	81.303	10.589	10.782	1.00	63.95	D
	ATOM	5703	NZ	LYS	D	271	82.195	9.772	11.664	1.00	62.34	D
	ATOM	5704	C	LYS	D	271	80.146	10.607	15.114	1.00	56.61	D
	ATOM	5705	O	LYS	D	271	79.604	11.715	15.119	1.00	56.97	D
	ATOM	5706	N	ARG	D	272	81.403	10.412	15.483	1.00	53.78	D
40	ATOM	5707	CA	ARG	D	272	82.212	11.531	15.902	1.00	51.25	D
	ATOM	5708	CB	ARG	D	272	81.625	12.153	17.159	1.00	50.62	D
	ATOM	5709	CG	ARG	D	272	81.295	13.617	16.977	1.00	50.35	D
	ATOM	5710	CD	ARG	D	272	82.497	14.465	17.304	1.00	50.29	D
	ATOM	5711	NE	ARG	D	272	82.835	15.461	16.290	1.00	50.91	D
45	ATOM	5712	CZ	ARG	D	272	82.084	16.507	15.950	1.00	50.34	D
	ATOM	5713	NH1	ARG	D	272	80.913	16.720	16.528	1.00	50.37	D
	ATOM	5714	NH2	ARG	D	272	82.528	17.376	15.049	1.00	50.67	D
	ATOM	5715	C	ARG	D	272	83.652	11.142	16.124	1.00	49.27	D
	ATOM	5716	O	ARG	D	272	83.995	10.497	17.112	1.00	50.77	D
50	ATOM	5717	N	ASP	D	273	84.498	11.523	15.180	1.00	45.44	D
	ATOM	5718	CA	ASP	D	273	85.904	11.229	15.310	1.00	40.81	D
	ATOM	5719	CB	ASP	D	273	86.582	11.281	13.951	1.00	40.44	D
	ATOM	5720	CG	ASP	D	273	87.998	10.765	13.997	1.00	40.32	D
	ATOM	5721	OD1	ASP	D	273	88.731	11.138	14.939	1.00	40.48	D

	ATOM	5722	OD2	ASP	D	273	88.377	9.991	13.094	1.00	40.70	D
	ATOM	5723	C	ASP	D	273	86.486	12.295	16.231	1.00	38.02	D
	ATOM	5724	O	ASP	D	273	87.082	13.269	15.771	1.00	36.97	D
5	ATOM	5725	N	LEU	D	274	86.301	12.096	17.536	1.00	35.35	D
	ATOM	5726	CA	LEU	D	274	86.783	13.026	18.562	1.00	32.44	D
	ATOM	5727	CB	LEU	D	274	86.596	12.405	19.957	1.00	32.29	D
	ATOM	5728	CG	LEU	D	274	85.237	11.729	20.146	1.00	33.44	D
	ATOM	5729	CD1	LEU	D	274	85.148	10.949	21.454	1.00	33.06	D
10	ATOM	5730	CD2	LEU	D	274	84.185	12.796	20.076	1.00	33.99	D
	ATOM	5731	C	LEU	D	274	88.250	13.443	18.376	1.00	30.29	D
	ATOM	5732	O	LEU	D	274	88.589	14.620	18.487	1.00	29.35	D
	ATOM	5733	N	ILE	D	275	89.119	12.481	18.090	1.00	27.97	D
	ATOM	5734	CA	ILE	D	275	90.529	12.790	17.919	1.00	26.53	D
15	ATOM	5735	CB	ILE	D	275	91.366	11.487	17.721	1.00	26.41	D
	ATOM	5736	CG2	ILE	D	275	92.798	11.829	17.316	1.00	25.43	D
	ATOM	5737	CG1	ILE	D	275	91.390	10.679	19.029	1.00	24.46	D
	ATOM	5738	CD1	ILE	D	275	92.026	11.404	20.207	1.00	19.75	D
	ATOM	5739	C	ILE	D	275	90.738	13.764	16.748	1.00	26.48	D
20	ATOM	5740	O	ILE	D	275	91.490	14.743	16.855	1.00	26.90	D
	ATOM	5741	N	THR	D	276	90.052	13.503	15.642	1.00	24.10	D
	ATOM	5742	CA	THR	D	276	90.134	14.348	14.469	1.00	22.65	D
	ATOM	5743	CB	THR	D	276	89.447	13.632	13.273	1.00	21.40	D
	ATOM	5744	OG1	THR	D	276	90.221	12.483	12.942	1.00	21.35	D
25	ATOM	5745	CG2	THR	D	276	89.321	14.528	12.052	1.00	18.26	D
	ATOM	5746	C	THR	D	276	89.477	15.711	14.769	1.00	23.50	D
	ATOM	5747	O	THR	D	276	90.041	16.768	14.462	1.00	22.31	D
	ATOM	5748	N	SER	D	277	88.305	15.673	15.397	1.00	23.60	D
	ATOM	5749	CA	SER	D	277	87.582	16.883	15.745	1.00	25.64	D
30	ATOM	5750	CB	SER	D	277	86.156	16.544	16.144	1.00	25.38	D
	ATOM	5751	OG	SER	D	277	85.440	16.087	15.019	1.00	27.48	D
	ATOM	5752	C	SER	D	277	88.215	17.739	16.837	1.00	26.65	D
	ATOM	5753	O	SER	D	277	88.380	18.939	16.657	1.00	29.61	D
	ATOM	5754	N	LEU	D	278	88.561	17.147	17.970	1.00	25.91	D
35	ATOM	5755	CA	LEU	D	278	89.180	17.922	19.035	1.00	26.38	D
	ATOM	5756	CB	LEU	D	278	89.564	17.027	20.218	1.00	26.10	D
	ATOM	5757	CG	LEU	D	278	88.426	16.811	21.194	1.00	24.98	D
	ATOM	5758	CD1	LEU	D	278	88.017	18.153	21.792	1.00	26.21	D
	ATOM	5759	CD2	LEU	D	278	87.257	16.190	20.458	1.00	28.73	D
40	ATOM	5760	C	LEU	D	278	90.426	18.621	18.530	1.00	26.46	D
	ATOM	5761	O	LEU	D	278	91.038	18.189	17.549	1.00	27.90	D
	ATOM	5762	N	PRO	D	279	90.803	19.733	19.177	1.00	26.62	D
	ATOM	5763	CD	PRO	D	279	89.970	20.521	20.096	1.00	26.92	D
	ATOM	5764	CA	PRO	D	279	91.994	20.496	18.799	1.00	27.49	D
	ATOM	5765	CB	PRO	D	279	91.940	21.686	19.739	1.00	26.12	D
45	ATOM	5766	CG	PRO	D	279	90.495	21.922	19.861	1.00	25.59	D
	ATOM	5767	C	PRO	D	279	93.212	19.620	19.047	1.00	29.22	D
	ATOM	5768	O	PRO	D	279	93.221	18.827	19.991	1.00	30.55	D
	ATOM	5769	N	PHE	D	280	94.234	19.775	18.210	1.00	29.38	D
50	ATOM	5770	CA	PHE	D	280	95.452	18.980	18.303	1.00	29.08	D
	ATOM	5771	CB	PHE	D	280	96.567	19.668	17.518	1.00	30.38	D
	ATOM	5772	CG	PHE	D	280	97.839	18.871	17.438	1.00	33.85	D
	ATOM	5773	CD1	PHE	D	280	97.849	17.585	16.890	1.00	35.64	D
	ATOM	5774	CD2	PHE	D	280	99.038	19.415	17.886	1.00	34.62	D
	ATOM	5775	CE1	PHE	D	280	99.045	16.852	16.789	1.00	36.28	D

	ATOM	5776	CE2	PHE	D	280	100.237	18.696	17.790	1.00	35.86	D
	ATOM	5777	CZ	PHE	D	280	100.242	17.410	17.239	1.00	36.27	D
	ATOM	5778	C	PHE	D	280	95.883	18.747	19.746	1.00	28.87	D
	ATOM	5779	O	PHE	D	280	96.100	17.611	20.167	1.00	28.22	D
5	ATOM	5780	N	GLU	D	281	95.977	19.824	20.513	1.00	29.70	D
	ATOM	5781	CA	GLU	D	281	96.394	19.735	21.906	1.00	30.73	D
	ATOM	5782	CB	GLU	D	281	96.367	21.124	22.544	1.00	30.74	D
	ATOM	5783	CG	GLU	D	281	96.958	22.225	21.686	1.00	35.82	D
	ATOM	5784	CD	GLU	D	281	96.181	22.455	20.365	1.00	39.11	D
10	ATOM	5785	OE1	GLU	D	281	94.927	22.371	20.364	1.00	37.33	D
	ATOM	5786	OE2	GLU	D	281	96.838	22.734	19.329	1.00	41.78	D
	ATOM	5787	C	GLU	D	281	95.508	18.767	22.707	1.00	30.47	D
	ATOM	5788	O	GLU	D	281	95.998	17.800	23.291	1.00	29.60	D
	ATOM	5789	N	ILE	D	282	94.200	19.006	22.731	1.00	30.62	D
15	ATOM	5790	CA	ILE	D	282	93.326	18.115	23.495	1.00	30.51	D
	ATOM	5791	CB	ILE	D	282	91.826	18.479	23.367	1.00	28.68	D
	ATOM	5792	CG2	ILE	D	282	90.973	17.454	24.096	1.00	25.40	D
	ATOM	5793	CG1	ILE	D	282	91.559	19.841	24.002	1.00	28.37	D
	ATOM	5794	CD1	ILE	D	282	92.338	20.960	23.374	1.00	29.50	D
20	ATOM	5795	C	ILE	D	282	93.506	16.667	23.085	1.00	30.93	D
	ATOM	5796	O	ILE	D	282	93.569	15.798	23.939	1.00	32.03	D
	ATOM	5797	N	SER	D	283	93.597	16.403	21.786	1.00	33.38	D
	ATOM	5798	CA	SER	D	283	93.773	15.037	21.315	1.00	33.57	D
	ATOM	5799	CB	SER	D	283	93.729	14.991	19.793	1.00	33.09	D
25	ATOM	5800	OG	SER	D	283	92.440	14.625	19.343	1.00	33.69	D
	ATOM	5801	C	SER	D	283	95.060	14.383	21.806	1.00	34.43	D
	ATOM	5802	O	SER	D	283	95.102	13.171	21.996	1.00	35.71	D
	ATOM	5803	N	LEU	D	284	96.121	15.158	21.996	1.00	33.67	D
	ATOM	5804	CA	LEU	D	284	97.345	14.541	22.479	1.00	33.99	D
30	ATOM	5805	CB	LEU	D	284	98.511	15.514	22.412	1.00	34.78	D
	ATOM	5806	CG	LEU	D	284	98.908	15.828	20.966	1.00	37.92	D
	ATOM	5807	CD1	LEU	D	284	99.965	16.921	20.972	1.00	38.44	D
	ATOM	5808	CD2	LEU	D	284	99.424	14.571	20.264	1.00	35.81	D
	ATOM	5809	C	LEU	D	284	97.105	14.089	23.908	1.00	34.14	D
35	ATOM	5810	O	LEU	D	284	97.469	12.972	24.268	1.00	35.96	D
	ATOM	5811	N	LYS	D	285	96.470	14.944	24.710	1.00	32.83	D
	ATOM	5812	CA	LYS	D	285	96.180	14.598	26.094	1.00	31.02	D
	ATOM	5813	CB	LYS	D	285	95.192	15.590	26.711	1.00	32.29	D
	ATOM	5814	CG	LYS	D	285	95.694	17.027	26.672	1.00	34.86	D
40	ATOM	5815	CD	LYS	D	285	94.977	17.944	27.659	1.00	38.81	D
	ATOM	5816	CE	LYS	D	285	95.626	17.931	29.043	1.00	41.32	D
	ATOM	5817	NZ	LYS	D	285	95.083	19.055	29.866	1.00	43.73	D
	ATOM	5818	C	LYS	D	285	95.603	13.194	26.129	1.00	28.79	D
	ATOM	5819	O	LYS	D	285	96.124	12.305	26.823	1.00	29.62	D
45	ATOM	5820	N	ILE	D	286	94.538	12.991	25.360	1.00	25.19	D
	ATOM	5821	CA	ILE	D	286	93.898	11.681	25.281	1.00	24.05	D
	ATOM	5822	CB	ILE	D	286	92.834	11.660	24.148	1.00	22.82	D
	ATOM	5823	CG2	ILE	D	286	92.176	10.291	24.060	1.00	21.24	D
	ATOM	5824	CG1	ILE	D	286	91.800	12.757	24.414	1.00	23.94	D
50	ATOM	5825	CD1	ILE	D	286	90.731	12.886	23.321	1.00	23.24	D
	ATOM	5826	C	ILE	D	286	94.950	10.583	25.036	1.00	23.79	D
	ATOM	5827	O	ILE	D	286	94.970	9.573	25.738	1.00	22.04	D
	ATOM	5828	N	PHE	D	287	95.825	10.788	24.051	1.00	21.07	D
	ATOM	5829	CA	PHE	D	287	96.844	9.790	23.746	1.00	21.11	D

	ATOM	5830	CB	PHE	D	287	97.596	10.147	22.469	1.00	20.53	D
	ATOM	5831	CG	PHE	D	287	96.842	9.818	21.221	1.00	20.94	D
	ATOM	5832	CD1	PHE	D	287	96.528	8.495	20.915	1.00	18.61	D
	ATOM	5833	CD2	PHE	D	287	96.445	10.831	20.340	1.00	20.85	D
5	ATOM	5834	CE1	PHE	D	287	95.835	8.184	19.754	1.00	17.26	D
	ATOM	5835	CE2	PHE	D	287	95.752	10.525	19.177	1.00	18.21	D
	ATOM	5836	CZ	PHE	D	287	95.444	9.204	18.876	1.00	16.07	D
	ATOM	5837	C	PHE	D	287	97.849	9.539	24.859	1.00	21.96	D
	ATOM	5838	O	PHE	D	287	98.314	8.418	25.035	1.00	20.26	D
10	ATOM	5839	N	ASN	D	288	98.182	10.592	25.593	1.00	23.06	D
	ATOM	5840	CA	ASN	D	288	99.128	10.494	26.677	1.00	25.24	D
	ATOM	5841	CB	ASN	D	288	99.598	11.892	27.089	1.00	25.50	D
	ATOM	5842	CG	ASN	D	288	100.691	12.432	26.166	1.00	27.45	D
	ATOM	5843	OD1	ASN	D	288	101.539	11.660	25.680	1.00	29.10	D
15	ATOM	5844	ND2	ASN	D	288	100.696	13.750	25.936	1.00	25.61	D
	ATOM	5845	C	ASN	D	288	98.585	9.695	27.883	1.00	28.89	D
	ATOM	5846	O	ASN	D	288	99.331	9.376	28.815	1.00	28.16	D
	ATOM	5847	N	TYR	D	289	97.289	9.368	27.846	1.00	30.81	D
	ATOM	5848	CA	TYR	D	289	96.633	8.560	28.879	1.00	33.41	D
20	ATOM	5849	CB	TYR	D	289	95.210	9.038	29.193	1.00	35.09	D
	ATOM	5850	CG	TYR	D	289	95.100	10.237	30.098	1.00	38.19	D
	ATOM	5851	CD1	TYR	D	289	95.713	10.256	31.343	1.00	37.23	D
	ATOM	5852	CE1	TYR	D	289	95.585	11.353	32.182	1.00	37.83	D
	ATOM	5853	CD2	TYR	D	289	94.353	11.348	29.713	1.00	38.71	D
25	ATOM	5854	CE2	TYR	D	289	94.219	12.447	30.543	1.00	39.19	D
	ATOM	5855	CZ	TYR	D	289	94.838	12.449	31.778	1.00	38.07	D
	ATOM	5856	OH	TYR	D	289	94.716	13.558	32.596	1.00	37.65	D
	ATOM	5857	C	TYR	D	289	96.496	7.129	28.375	1.00	34.42	D
	ATOM	5858	O	TYR	D	289	95.852	6.288	29.016	1.00	34.85	D
30	ATOM	5859	N	LEU	D	290	97.076	6.857	27.215	1.00	34.95	D
	ATOM	5860	CA	LEU	D	290	96.980	5.530	26.632	1.00	36.71	D
	ATOM	5861	CB	LEU	D	290	96.488	5.621	25.189	1.00	37.91	D
	ATOM	5862	CG	LEU	D	290	95.004	5.925	24.991	1.00	38.82	D
	ATOM	5863	CD1	LEU	D	290	94.740	6.136	23.516	1.00	39.93	D
35	ATOM	5864	CD2	LEU	D	290	94.159	4.764	25.535	1.00	37.72	D
	ATOM	5865	C	LEU	D	290	98.302	4.802	26.664	1.00	37.19	D
	ATOM	5866	O	LEU	D	290	99.354	5.419	26.628	1.00	37.91	D
	ATOM	5867	N	GLN	D	291	98.256	3.482	26.744	1.00	38.53	D
	ATOM	5868	CA	GLN	D	291	99.493	2.736	26.771	1.00	39.34	D
40	ATOM	5869	CB	GLN	D	291	99.251	1.308	27.236	1.00	40.51	D
	ATOM	5870	CG	GLN	D	291	98.786	1.213	28.657	1.00	43.34	D
	ATOM	5871	CD	GLN	D	291	98.666	-0.215	29.102	1.00	46.99	D
	ATOM	5872	OE1	GLN	D	291	99.662	-0.945	29.172	1.00	50.86	D
	ATOM	5873	NE2	GLN	D	291	97.444	-0.638	29.398	1.00	49.26	D
45	ATOM	5874	C	GLN	D	291	100.090	2.749	25.374	1.00	38.68	D
	ATOM	5875	O	GLN	D	291	99.393	2.990	24.383	1.00	39.01	D
	ATOM	5876	N	PHE	D	292	101.386	2.482	25.308	1.00	35.62	D
	ATOM	5877	CA	PHE	D	292	102.096	2.492	24.059	1.00	32.95	D
	ATOM	5878	CB	PHE	D	292	103.583	2.209	24.335	1.00	32.02	D
50	ATOM	5879	CG	PHE	D	292	104.010	0.795	24.109	1.00	29.67	D
	ATOM	5880	CD1	PHE	D	292	104.290	0.349	22.829	1.00	30.05	D
	ATOM	5881	CD2	PHE	D	292	104.221	-0.064	25.176	1.00	29.27	D
	ATOM	5882	CE1	PHE	D	292	104.788	-0.932	22.613	1.00	30.66	D
	ATOM	5883	CE2	PHE	D	292	104.719	-1.348	24.972	1.00	29.01	D

	ATOM	5884	CZ	PHE	D	292	105.004	-1.781	23.686	1.00	29.86	D
	ATOM	5885	C	PHE	D	292	101.477	1.552	23.035	1.00	32.44	D
	ATOM	5886	O	PHE	D	292	101.384	1.894	21.852	1.00	33.62	D
	ATOM	5887	N	GLU	D	293	101.018	0.389	23.481	1.00	31.32	D
5	ATOM	5888	CA	GLU	D	293	100.396	-0.551	22.560	1.00	29.89	D
	ATOM	5889	CB	GLU	D	293	99.974	-1.819	23.296	1.00	29.10	D
	ATOM	5890	CG	GLU	D	293	101.135	-2.712	23.586	1.00	30.44	D
	ATOM	5891	CD	GLU	D	293	101.534	-2.717	25.053	1.00	31.93	D
	ATOM	5892	OE1	GLU	D	293	101.473	-1.647	25.722	1.00	28.98	D
10	ATOM	5893	OE2	GLU	D	293	101.924	-3.815	25.518	1.00	32.42	D
	ATOM	5894	C	GLU	D	293	99.187	0.044	21.864	1.00	28.52	D
	ATOM	5895	O	GLU	D	293	98.978	-0.193	20.679	1.00	26.63	D
	ATOM	5896	N	ASP	D	294	98.391	0.802	22.615	1.00	29.50	D
	ATOM	5897	CA	ASP	D	294	97.193	1.431	22.081	1.00	30.32	D
15	ATOM	5898	CB	ASP	D	294	96.330	2.030	23.210	1.00	32.63	D
	ATOM	5899	CG	ASP	D	294	95.768	0.968	24.183	1.00	36.82	D
	ATOM	5900	OD1	ASP	D	294	95.503	-0.192	23.772	1.00	39.44	D
	ATOM	5901	OD2	ASP	D	294	95.563	1.309	25.369	1.00	38.44	D
	ATOM	5902	C	ASP	D	294	97.585	2.542	21.103	1.00	29.40	D
20	ATOM	5903	O	ASP	D	294	96.796	2.930	20.245	1.00	27.84	D
	ATOM	5904	N	ILE	D	295	98.805	3.050	21.237	1.00	28.17	D
	ATOM	5905	CA	ILE	D	295	99.266	4.114	20.362	1.00	28.34	D
	ATOM	5906	CB	ILE	D	295	100.510	4.784	20.917	1.00	28.05	D
	ATOM	5907	CG2	ILE	D	295	100.845	5.998	20.077	1.00	25.51	D
25	ATOM	5908	CG1	ILE	D	295	100.294	5.145	22.392	1.00	30.16	D
	ATOM	5909	CD1	ILE	D	295	99.338	6.283	22.658	1.00	31.34	D
	ATOM	5910	C	ILE	D	295	99.605	3.549	18.990	1.00	28.98	D
	ATOM	5911	O	ILE	D	295	99.310	4.151	17.956	1.00	28.75	D
	ATOM	5912	N	ILE	D	296	100.227	2.381	18.996	1.00	29.17	D
30	ATOM	5913	CA	ILE	D	296	100.612	1.715	17.768	1.00	30.36	D
	ATOM	5914	CB	ILE	D	296	101.521	0.491	18.085	1.00	30.31	D
	ATOM	5915	CG2	ILE	D	296	101.236	-0.660	17.148	1.00	28.53	D
	ATOM	5916	CG1	ILE	D	296	102.987	0.911	17.989	1.00	31.04	D
	ATOM	5917	CD1	ILE	D	296	103.353	2.115	18.829	1.00	32.07	D
35	ATOM	5918	C	ILE	D	296	99.379	1.308	16.965	1.00	30.74	D
	ATOM	5919	O	ILE	D	296	99.376	1.398	15.741	1.00	30.48	D
	ATOM	5920	N	ASN	D	297	98.330	0.865	17.642	1.00	31.12	D
	ATOM	5921	CA	ASN	D	297	97.121	0.506	16.924	1.00	33.08	D
	ATOM	5922	CB	ASN	D	297	96.096	-0.099	17.865	1.00	33.38	D
40	ATOM	5923	CG	ASN	D	297	96.393	-1.537	18.171	1.00	37.25	D
	ATOM	5924	OD1	ASN	D	297	95.953	-2.067	19.194	1.00	37.85	D
	ATOM	5925	ND2	ASN	D	297	97.143	-2.196	17.270	1.00	37.30	D
	ATOM	5926	C	ASN	D	297	96.548	1.767	16.316	1.00	33.81	D
	ATOM	5927	O	ASN	D	297	96.220	1.817	15.123	1.00	34.30	D
45	ATOM	5928	N	SER	D	298	96.435	2.780	17.168	1.00	32.14	D
	ATOM	5929	CA	SER	D	298	95.912	4.079	16.792	1.00	30.45	D
	ATOM	5930	CB	SER	D	298	96.100	5.073	17.939	1.00	29.96	D
	ATOM	5931	OG	SER	D	298	95.395	4.648	19.087	1.00	27.42	D
	ATOM	5932	C	SER	D	298	96.656	4.566	15.583	1.00	30.58	D
50	ATOM	5933	O	SER	D	298	96.103	5.255	14.731	1.00	32.34	D
	ATOM	5934	N	LEU	D	299	97.930	4.216	15.514	1.00	29.49	D
	ATOM	5935	CA	LEU	D	299	98.738	4.628	14.387	1.00	28.00	D
	ATOM	5936	CB	LEU	D	299	100.164	4.131	14.570	1.00	28.12	D
	ATOM	5937	CG	LEU	D	299	101.291	5.098	14.240	1.00	28.83	D

	ATOM	5938	CD1	LEU	D	299	101.105	6.442	14.938	1.00	28.49	D
	ATOM	5939	CD2	LEU	D	299	102.595	4.455	14.703	1.00	30.72	D
	ATOM	5940	C	LEU	D	299	98.147	4.063	13.108	1.00	27.04	D
	ATOM	5941	O	LEU	D	299	98.382	4.608	12.045	1.00	28.76	D
5	ATOM	5942	N	GLY	D	300	97.356	2.996	13.212	1.00	25.60	D
	ATOM	5943	CA	GLY	D	300	96.783	2.387	12.018	1.00	25.16	D
	ATOM	5944	C	GLY	D	300	95.268	2.423	11.857	1.00	25.49	D
	ATOM	5945	O	GLY	D	300	94.665	1.528	11.258	1.00	24.96	D
	ATOM	5946	N	VAL	D	301	94.661	3.476	12.381	1.00	26.14	D
10	ATOM	5947	CA	VAL	D	301	93.223	3.677	12.335	1.00	25.65	D
	ATOM	5948	CB	VAL	D	301	92.783	4.425	13.635	1.00	25.13	D
	ATOM	5949	CG1	VAL	D	301	91.377	4.975	13.523	1.00	23.49	D
	ATOM	5950	CG2	VAL	D	301	92.881	3.470	14.818	1.00	25.09	D
	ATOM	5951	C	VAL	D	301	92.853	4.482	11.085	1.00	26.83	D
15	ATOM	5952	O	VAL	D	301	91.895	4.160	10.386	1.00	29.06	D
	ATOM	5953	N	SER	D	302	93.624	5.517	10.781	1.00	27.15	D
	ATOM	5954	CA	SER	D	302	93.321	6.327	9.611	1.00	27.14	D
	ATOM	5955	CB	SER	D	302	92.021	7.096	9.832	1.00	26.96	D
	ATOM	5956	OG	SER	D	302	92.186	8.048	10.876	1.00	28.29	D
20	ATOM	5957	C	SER	D	302	94.442	7.308	9.329	1.00	26.93	D
	ATOM	5958	O	SER	D	302	95.174	7.696	10.239	1.00	27.64	D
	ATOM	5959	N	GLN	D	303	94.558	7.720	8.067	1.00	26.82	D
	ATOM	5960	CA	GLN	D	303	95.596	8.658	7.661	1.00	25.04	D
	ATOM	5961	CB	GLN	D	303	95.362	9.166	6.244	1.00	23.83	D
25	ATOM	5962	CG	GLN	D	303	95.865	8.261	5.154	1.00	29.99	D
	ATOM	5963	CD	GLN	D	303	97.398	8.160	5.090	1.00	32.84	D
	ATOM	5964	OE1	GLN	D	303	97.942	7.457	4.239	1.00	34.49	D
	ATOM	5965	NE2	GLN	D	303	98.091	8.863	5.986	1.00	36.06	D
	ATOM	5966	C	GLN	D	303	95.653	9.852	8.587	1.00	23.97	D
30	ATOM	5967	O	GLN	D	303	96.743	10.343	8.901	1.00	22.53	D
	ATOM	5968	N	ASN	D	304	94.490	10.322	9.034	1.00	22.85	D
	ATOM	5969	CA	ASN	D	304	94.479	11.487	9.908	1.00	24.54	D
	ATOM	5970	CB	ASN	D	304	93.082	12.042	10.095	1.00	25.34	D
	ATOM	5971	CG	ASN	D	304	93.105	13.358	10.814	1.00	28.24	D
35	ATOM	5972	OD1	ASN	D	304	92.215	13.657	11.613	1.00	30.04	D
	ATOM	5973	ND2	ASN	D	304	94.143	14.163	10.544	1.00	29.46	D
	ATOM	5974	C	ASN	D	304	95.058	11.172	11.270	1.00	25.25	D
	ATOM	5975	O	ASN	D	304	95.876	11.928	11.820	1.00	24.93	D
	ATOM	5976	N	TRP	D	305	94.609	10.063	11.835	1.00	25.15	D
40	ATOM	5977	CA	TRP	D	305	95.139	9.658	13.118	1.00	25.51	D
	ATOM	5978	CB	TRP	D	305	94.447	8.373	13.587	1.00	25.43	D
	ATOM	5979	CG	TRP	D	305	93.138	8.630	14.311	1.00	26.00	D
	ATOM	5980	CD2	TRP	D	305	92.614	7.880	15.410	1.00	26.49	D
	ATOM	5981	CE2	TRP	D	305	91.351	8.425	15.730	1.00	24.97	D
45	ATOM	5982	CE3	TRP	D	305	93.090	6.796	16.157	1.00	27.62	D
	ATOM	5983	CD1	TRP	D	305	92.199	9.581	14.015	1.00	25.09	D
	ATOM	5984	NE1	TRP	D	305	91.122	9.461	14.864	1.00	24.10	D
	ATOM	5985	CZ2	TRP	D	305	90.559	7.918	16.764	1.00	23.76	D
	ATOM	5986	CZ3	TRP	D	305	92.299	6.297	17.183	1.00	25.00	D
50	ATOM	5987	CH2	TRP	D	305	91.053	6.859	17.474	1.00	24.03	D
	ATOM	5988	C	TRP	D	305	96.656	9.477	12.935	1.00	24.69	D
	ATOM	5989	O	TRP	D	305	97.445	9.992	13.734	1.00	25.68	D
	ATOM	5990	N	ASN	D	306	97.054	8.786	11.863	1.00	22.23	D
	ATOM	5991	CA	ASN	D	306	98.471	8.583	11.555	1.00	21.36	D

	ATOM	5992	CB	ASN	D	306	98.669	7.946	10.182	1.00	19.88	D
	ATOM	5993	CG	ASN	D	306	100.134	7.572	9.920	1.00	20.62	D
	ATOM	5994	OD1	ASN	D	306	100.608	6.526	10.394	1.00	21.63	D
	ATOM	5995	ND2	ASN	D	306	100.860	8.427	9.176	1.00	16.92	D
5	ATOM	5996	C	ASN	D	306	99.203	9.913	11.517	1.00	21.93	D
	ATOM	5997	O	ASN	D	306	100.356	10.009	11.912	1.00	21.70	D
	ATOM	5998	N	LYS	D	307	98.533	10.930	11.000	1.00	22.01	D
	ATOM	5999	CA	LYS	D	307	99.134	12.235	10.907	1.00	23.12	D
	ATOM	6000	CB	LYS	D	307	98.270	13.136	10.027	1.00	24.42	D
10	ATOM	6001	CG	LYS	D	307	98.897	14.469	9.657	1.00	25.07	D
	ATOM	6002	CD	LYS	D	307	97.803	15.504	9.446	1.00	29.41	D
	ATOM	6003	CE	LYS	D	307	98.290	16.723	8.650	1.00	31.20	D
	ATOM	6004	NZ	LYS	D	307	98.710	16.351	7.251	1.00	30.25	D
	ATOM	6005	C	LYS	D	307	99.298	12.868	12.284	1.00	24.28	D
15	ATOM	6006	O	LYS	D	307	100.387	13.292	12.654	1.00	26.10	D
	ATOM	6007	N	ILE	D	308	98.214	12.902	13.047	1.00	23.74	D
	ATOM	6008	CA	ILE	D	308	98.217	13.520	14.359	1.00	25.31	D
	ATOM	6009	CB	ILE	D	308	96.843	13.350	15.042	1.00	27.23	D
	ATOM	6010	CG2	ILE	D	308	96.899	13.810	16.475	1.00	27.28	D
20	ATOM	6011	CG1	ILE	D	308	95.794	14.187	14.294	1.00	28.70	D
	ATOM	6012	CD1	ILE	D	308	94.383	14.048	14.808	1.00	26.95	D
	ATOM	6013	C	ILE	D	308	99.298	13.018	15.292	1.00	25.96	D
	ATOM	6014	O	ILE	D	308	100.079	13.797	15.838	1.00	24.81	D
	ATOM	6015	N	ILE	D	309	99.353	11.710	15.464	1.00	26.12	D
25	ATOM	6016	CA	ILE	D	309	100.314	11.115	16.359	1.00	25.75	D
	ATOM	6017	CB	ILE	D	309	99.990	9.603	16.538	1.00	25.30	D
	ATOM	6018	CG2	ILE	D	309	100.995	8.937	17.437	1.00	24.21	D
	ATOM	6019	CG1	ILE	D	309	98.617	9.437	17.181	1.00	21.52	D
	ATOM	6020	CD1	ILE	D	309	98.160	8.023	17.261	1.00	23.28	D
30	ATOM	6021	C	ILE	D	309	101.755	11.313	15.906	1.00	26.74	D
	ATOM	6022	O	ILE	D	309	102.626	11.586	16.729	1.00	27.84	D
	ATOM	6023	N	ARG	D	310	102.026	11.177	14.610	1.00	28.38	D
	ATOM	6024	CA	ARG	D	310	103.401	11.350	14.098	1.00	29.18	D
	ATOM	6025	CB	ARG	D	310	103.513	10.811	12.663	1.00	28.52	D
35	ATOM	6026	CG	ARG	D	310	103.531	9.277	12.560	1.00	30.67	D
	ATOM	6027	CD	ARG	D	310	103.052	8.787	11.186	1.00	34.25	D
	ATOM	6028	NE	ARG	D	310	104.098	8.252	10.323	1.00	36.16	D
	ATOM	6029	CZ	ARG	D	310	105.097	8.969	9.827	1.00	38.55	D
	ATOM	6030	NH1	ARG	D	310	105.200	10.259	10.095	1.00	42.20	D
40	ATOM	6031	NH2	ARG	D	310	106.009	8.391	9.069	1.00	41.89	D
	ATOM	6032	C	ARG	D	310	103.838	12.811	14.139	1.00	28.88	D
	ATOM	6033	O	ARG	D	310	104.996	13.133	13.873	1.00	28.32	D
	ATOM	6034	N	LYS	D	311	102.900	13.681	14.496	1.00	29.76	D
	ATOM	6035	CA	LYS	D	311	103.172	15.104	14.570	1.00	32.11	D
45	ATOM	6036	CB	LYS	D	311	101.894	15.868	14.227	1.00	32.03	D
	ATOM	6037	CG	LYS	D	311	102.061	17.362	14.098	1.00	36.15	D
	ATOM	6038	CD	LYS	D	311	100.731	18.049	13.814	1.00	39.43	D
	ATOM	6039	CE	LYS	D	311	100.895	19.580	13.814	1.00	42.31	D
	ATOM	6040	NZ	LYS	D	311	100.575	20.231	15.122	1.00	42.00	D
50	ATOM	6041	C	LYS	D	311	103.728	15.564	15.934	1.00	32.85	D
	ATOM	6042	O	LYS	D	311	104.467	16.545	15.992	1.00	32.33	D
	ATOM	6043	N	SER	D	312	103.395	14.855	17.017	1.00	33.76	D
	ATOM	6044	CA	SER	D	312	103.857	15.223	18.365	1.00	33.60	D
	ATOM	6045	CB	SER	D	312	102.835	14.787	19.421	1.00	35.34	D

5	ATOM	6046	OG	SER	D	312	103.198	15.271	20.712	1.00	39.47	D
	ATOM	6047	C	SER	D	312	105.222	14.667	18.781	1.00	31.68	D
	ATOM	6048	O	SER	D	312	105.456	13.468	18.728	1.00	32.40	D
	ATOM	6049	N	THR	D	313	106.125	15.543	19.198	1.00	30.17	D
	ATOM	6050	CA	THR	D	313	107.429	15.095	19.651	1.00	29.28	D
10	ATOM	6051	CB	THR	D	313	108.502	16.214	19.480	1.00	30.08	D
	ATOM	6052	OG1	THR	D	313	109.122	16.072	18.199	1.00	31.16	D
	ATOM	6053	CG2	THR	D	313	109.580	16.132	20.558	1.00	30.05	D
	ATOM	6054	C	THR	D	313	107.270	14.701	21.128	1.00	27.77	D
	ATOM	6055	O	THR	D	313	107.658	13.603	21.538	1.00	26.51	D
15	ATOM	6056	N	SER	D	314	106.666	15.599	21.901	1.00	26.12	D
	ATOM	6057	CA	SER	D	314	106.420	15.370	23.311	1.00	26.42	D
	ATOM	6058	CB	SER	D	314	105.499	16.454	23.886	1.00	25.86	D
	ATOM	6059	OG	SER	D	314	104.133	16.191	23.589	1.00	25.20	D
	ATOM	6060	C	SER	D	314	105.755	14.011	23.534	1.00	26.86	D
20	ATOM	6061	O	SER	D	314	106.064	13.314	24.486	1.00	27.19	D
	ATOM	6062	N	LEU	D	315	104.830	13.633	22.668	1.00	26.78	D
	ATOM	6063	CA	LEU	D	315	104.169	12.368	22.851	1.00	26.12	D
	ATOM	6064	CB	LEU	D	315	103.148	12.167	21.741	1.00	25.84	D
	ATOM	6065	CG	LEU	D	315	102.212	10.960	21.711	1.00	26.39	D
25	ATOM	6066	CD1	LEU	D	315	101.094	11.269	20.721	1.00	27.77	D
	ATOM	6067	CD2	LEU	D	315	102.933	9.691	21.303	1.00	24.47	D
	ATOM	6068	C	LEU	D	315	105.186	11.229	22.899	1.00	26.05	D
	ATOM	6069	O	LEU	D	315	105.108	10.373	23.780	1.00	27.85	D
	ATOM	6070	N	TRP	D	316	106.165	11.224	21.998	1.00	24.50	D
30	ATOM	6071	CA	TRP	D	316	107.141	10.138	22.011	1.00	25.89	D
	ATOM	6072	CB	TRP	D	316	107.751	9.952	20.607	1.00	24.16	D
	ATOM	6073	CG	TRP	D	316	106.708	9.452	19.635	1.00	21.27	D
	ATOM	6074	CD2	TRP	D	316	106.177	8.123	19.565	1.00	18.61	D
	ATOM	6075	CE2	TRP	D	316	105.107	8.146	18.646	1.00	18.90	D
35	ATOM	6076	CE3	TRP	D	316	106.498	6.917	20.193	1.00	20.19	D
	ATOM	6077	CD1	TRP	D	316	105.959	10.206	18.767	1.00	20.28	D
	ATOM	6078	NE1	TRP	D	316	104.994	9.428	18.177	1.00	19.42	D
	ATOM	6079	CZ2	TRP	D	316	104.351	7.007	18.344	1.00	19.58	D
	ATOM	6080	CZ3	TRP	D	316	105.741	5.778	19.892	1.00	21.16	D
40	ATOM	6081	CH2	TRP	D	316	104.682	5.835	18.975	1.00	20.34	D
	ATOM	6082	C	TRP	D	316	108.216	10.292	23.091	1.00	27.23	D
	ATOM	6083	O	TRP	D	316	108.854	9.311	23.519	1.00	27.64	D
	ATOM	6084	N	LYS	D	317	108.374	11.525	23.556	1.00	27.58	D
	ATOM	6085	CA	LYS	D	317	109.332	11.847	24.602	1.00	27.23	D
45	ATOM	6086	CB	LYS	D	317	109.463	13.360	24.759	1.00	29.14	D
	ATOM	6087	CG	LYS	D	317	110.589	13.760	25.682	1.00	32.80	D
	ATOM	6088	CD	LYS	D	317	110.743	15.264	25.749	1.00	35.26	D
	ATOM	6089	CE	LYS	D	317	111.774	15.652	26.805	1.00	37.31	D
	ATOM	6090	NZ	LYS	D	317	111.793	17.120	27.068	1.00	37.03	D
50	ATOM	6091	C	LYS	D	317	108.822	11.275	25.910	1.00	25.94	D
	ATOM	6092	O	LYS	D	317	109.570	10.685	26.689	1.00	25.94	D
	ATOM	6093	N	LYS	D	318	107.533	11.473	26.142	1.00	23.54	D
	ATOM	6094	CA	LYS	D	318	106.921	10.980	27.345	1.00	21.52	D
	ATOM	6095	CB	LYS	D	318	105.457	11.403	27.426	1.00	19.84	D
	ATOM	6096	CG	LYS	D	318	105.276	12.802	27.949	1.00	15.81	D
	ATOM	6097	CD	LYS	D	318	103.822	13.127	28.039	1.00	17.16	D
	ATOM	6098	CE	LYS	D	318	103.592	14.588	28.439	1.00	19.94	D
	ATOM	6099	NZ	LYS	D	318	104.446	15.524	27.676	1.00	22.18	D

	ATOM	6100	C	LYS	D	318	107.026	9.474	27.389	1.00	21.47	D
	ATOM	6101	O	LYS	D	318	107.353	8.890	28.423	1.00	22.72	D
	ATOM	6102	N	LEU	D	319	106.754	8.825	26.271	1.00	20.41	D
	ATOM	6103	CA	LEU	D	319	106.834	7.373	26.259	1.00	19.54	D
5	ATOM	6104	CB	LEU	D	319	106.427	6.839	24.894	1.00	17.41	D
	ATOM	6105	CG	LEU	D	319	104.933	6.610	24.750	1.00	14.60	D
	ATOM	6106	CD1	LEU	D	319	104.590	6.417	23.307	1.00	15.84	D
	ATOM	6107	CD2	LEU	D	319	104.520	5.398	25.581	1.00	13.04	D
	ATOM	6108	C	LEU	D	319	108.232	6.901	26.605	1.00	19.33	D
10	ATOM	6109	O	LEU	D	319	108.395	6.014	27.441	1.00	18.41	D
	ATOM	6110	N	LEU	D	320	109.239	7.493	25.961	1.00	20.82	D
	ATOM	6111	CA	LEU	D	320	110.624	7.099	26.217	1.00	21.24	D
	ATOM	6112	CB	LEU	D	320	111.589	7.926	25.344	1.00	17.94	D
	ATOM	6113	CG	LEU	D	320	111.710	7.492	23.869	1.00	18.89	D
15	ATOM	6114	CD1	LEU	D	320	112.467	8.533	23.030	1.00	16.82	D
	ATOM	6115	CD2	LEU	D	320	112.402	6.158	23.797	1.00	15.44	D
	ATOM	6116	C	LEU	D	320	110.965	7.259	27.701	1.00	22.18	D
	ATOM	6117	O	LEU	D	320	111.574	6.383	28.310	1.00	23.23	D
	ATOM	6118	N	ILE	D	321	110.545	8.375	28.281	1.00	22.59	D
20	ATOM	6119	CA	ILE	D	321	110.824	8.661	29.676	1.00	22.13	D
	ATOM	6120	CB	ILE	D	321	110.462	10.125	30.007	1.00	21.71	D
	ATOM	6121	CG2	ILE	D	321	110.406	10.336	31.509	1.00	20.64	D
	ATOM	6122	CG1	ILE	D	321	111.471	11.053	29.324	1.00	20.39	D
	ATOM	6123	CD1	ILE	D	321	111.312	12.527	29.639	1.00	17.62	D
25	ATOM	6124	C	ILE	D	321	110.112	7.729	30.641	1.00	21.87	D
	ATOM	6125	O	ILE	D	321	110.726	7.204	31.551	1.00	23.61	D
	ATOM	6126	N	SER	D	322	108.819	7.526	30.449	1.00	22.79	D
	ATOM	6127	CA	SER	D	322	108.082	6.663	31.345	1.00	23.92	D
	ATOM	6128	CB	SER	D	322	106.610	6.624	30.943	1.00	24.36	D
30	ATOM	6129	OG	SER	D	322	106.464	6.398	29.554	1.00	28.99	D
	ATOM	6130	C	SER	D	322	108.668	5.256	31.377	1.00	25.68	D
	ATOM	6131	O	SER	D	322	108.780	4.660	32.440	1.00	27.76	D
	ATOM	6132	N	GLU	D	323	109.041	4.718	30.222	1.00	24.70	D
	ATOM	6133	CA	GLU	D	323	109.625	3.389	30.188	1.00	23.55	D
35	ATOM	6134	CB	GLU	D	323	109.581	2.835	28.775	1.00	24.33	D
	ATOM	6135	CG	GLU	D	323	108.228	2.303	28.385	1.00	25.11	D
	ATOM	6136	CD	GLU	D	323	107.953	0.951	29.008	1.00	26.37	D
	ATOM	6137	OE1	GLU	D	323	108.775	0.024	28.805	1.00	26.30	D
	ATOM	6138	OE2	GLU	D	323	106.920	0.809	29.695	1.00	27.36	D
40	ATOM	6139	C	GLU	D	323	111.059	3.448	30.678	1.00	23.31	D
	ATOM	6140	O	GLU	D	323	111.773	2.443	30.684	1.00	23.15	D
	ATOM	6141	N	ASN	D	324	111.467	4.644	31.091	1.00	22.23	D
	ATOM	6142	CA	ASN	D	324	112.812	4.891	31.592	1.00	22.59	D
	ATOM	6143	CB	ASN	D	324	113.038	4.090	32.877	1.00	22.90	D
45	ATOM	6144	CG	ASN	D	324	111.864	4.200	33.858	1.00	26.71	D
	ATOM	6145	OD1	ASN	D	324	111.346	5.294	34.109	1.00	25.11	D
	ATOM	6146	ND2	ASN	D	324	111.450	3.056	34.430	1.00	28.34	D
	ATOM	6147	C	ASN	D	324	113.911	4.565	30.560	1.00	23.12	D
	ATOM	6148	O	ASN	D	324	114.971	4.031	30.914	1.00	23.08	D
50	ATOM	6149	N	PHE	D	325	113.667	4.881	29.285	1.00	22.49	D
	ATOM	6150	CA	PHE	D	325	114.673	4.613	28.246	1.00	22.20	D
	ATOM	6151	CB	PHE	D	325	114.005	4.332	26.882	1.00	18.54	D
	ATOM	6152	CG	PHE	D	325	113.296	2.991	26.806	1.00	18.28	D
	ATOM	6153	CD1	PHE	D	325	112.080	2.864	26.117	1.00	17.36	D

	ATOM	6154	CD2	PHE	D	325	113.828	1.860	27.425	1.00	17.01	D
	ATOM	6155	CE1	PHE	D	325	111.404	1.631	26.053	1.00	15.65	D
	ATOM	6156	CE2	PHE	D	325	113.165	0.617	27.369	1.00	16.41	D
	ATOM	6157	CZ	PHE	D	325	111.942	0.508	26.677	1.00	16.67	D
5	ATOM	6158	C	PHE	D	325	115.640	5.798	28.136	1.00	21.95	D
	ATOM	6159	O	PHE	D	325	116.735	5.686	27.578	1.00	21.44	D
	ATOM	6160	N	VAL	D	326	115.240	6.925	28.707	1.00	21.18	D
	ATOM	6161	CA	VAL	D	326	116.059	8.113	28.642	1.00	21.85	D
	ATOM	6162	CB	VAL	D	326	115.922	8.765	27.238	1.00	21.90	D
10	ATOM	6163	CG1	VAL	D	326	114.455	9.085	26.972	1.00	22.16	D
	ATOM	6164	CG2	VAL	D	326	116.772	10.016	27.133	1.00	19.90	D
	ATOM	6165	C	VAL	D	326	115.619	9.084	29.725	1.00	22.99	D
	ATOM	6166	O	VAL	D	326	114.453	9.105	30.121	1.00	23.26	D
	ATOM	6167	N	SER	D	327	116.571	9.869	30.215	1.00	26.57	D
15	ATOM	6168	CA	SER	D	327	116.308	10.853	31.257	1.00	30.18	D
	ATOM	6169	CB	SER	D	327	117.552	11.111	32.099	1.00	28.88	D
	ATOM	6170	OG	SER	D	327	117.794	10.061	33.008	1.00	34.20	D
	ATOM	6171	C	SER	D	327	115.914	12.167	30.648	1.00	32.93	D
	ATOM	6172	O	SER	D	327	116.304	12.488	29.533	1.00	33.50	D
20	ATOM	6173	N	PRO	D	328	115.141	12.958	31.384	1.00	36.30	D
	ATOM	6174	CD	PRO	D	328	114.483	12.591	32.644	1.00	38.28	D
	ATOM	6175	CA	PRO	D	328	114.693	14.269	30.923	1.00	38.59	D
	ATOM	6176	CB	PRO	D	328	113.988	14.834	32.140	1.00	38.19	D
	ATOM	6177	CG	PRO	D	328	113.360	13.609	32.728	1.00	39.16	D
25	ATOM	6178	C	PRO	D	328	115.900	15.110	30.526	1.00	40.86	D
	ATOM	6179	O	PRO	D	328	115.886	15.787	29.496	1.00	42.18	D
	ATOM	6180	N	LYS	D	329	116.955	15.053	31.332	1.00	41.28	D
	ATOM	6181	CA	LYS	D	329	118.143	15.826	31.027	1.00	42.86	D
	ATOM	6182	CB	LYS	D	329	118.861	16.228	32.327	1.00	46.62	D
30	ATOM	6183	CG	LYS	D	329	118.066	17.272	33.169	1.00	49.10	D
	ATOM	6184	CD	LYS	D	329	118.615	17.445	34.594	1.00	50.67	D
	ATOM	6185	CE	LYS	D	329	120.077	17.887	34.606	1.00	51.76	D
	ATOM	6186	NZ	LYS	D	329	120.645	17.988	35.993	1.00	51.50	D
	ATOM	6187	C	LYS	D	329	119.078	15.102	30.073	1.00	42.35	D
35	ATOM	6188	O	LYS	D	329	120.060	15.671	29.609	1.00	43.19	D
	ATOM	6189	N	GLY	D	330	118.766	13.850	29.765	1.00	41.86	D
	ATOM	6190	CA	GLY	D	330	119.597	13.107	28.837	1.00	40.87	D
	ATOM	6191	C	GLY	D	330	118.961	13.089	27.456	1.00	42.32	D
	ATOM	6192	O	GLY	D	330	119.470	12.461	26.528	1.00	41.14	D
40	ATOM	6193	N	PHE	D	331	117.849	13.798	27.304	1.00	44.29	D
	ATOM	6194	CA	PHE	D	331	117.148	13.809	26.026	1.00	46.40	D
	ATOM	6195	CB	PHE	D	331	115.887	14.660	26.119	1.00	47.33	D
	ATOM	6196	CG	PHE	D	331	114.896	14.396	25.016	1.00	49.12	D
	ATOM	6197	CD1	PHE	D	331	114.198	13.188	24.958	1.00	48.42	D
45	ATOM	6198	CD2	PHE	D	331	114.658	15.359	24.033	1.00	49.78	D
	ATOM	6199	CE1	PHE	D	331	113.273	12.942	23.939	1.00	48.28	D
	ATOM	6200	CE2	PHE	D	331	113.735	15.128	23.008	1.00	49.07	D
	ATOM	6201	CZ	PHE	D	331	113.042	13.917	22.958	1.00	49.05	D
	ATOM	6202	C	PHE	D	331	117.983	14.276	24.846	1.00	46.95	D
50	ATOM	6203	O	PHE	D	331	118.017	13.613	23.815	1.00	48.73	D
	ATOM	6204	N	ASN	D	332	118.651	15.414	24.997	1.00	47.11	D
	ATOM	6205	CA	ASN	D	332	119.477	15.972	23.932	1.00	46.02	D
	ATOM	6206	CB	ASN	D	332	120.255	17.161	24.463	1.00	47.82	D
	ATOM	6207	CG	ASN	D	332	119.497	18.440	24.335	1.00	49.50	D

	ATOM	6208	OD1	ASN	D	332	118.322	18.519	24.692	1.00	50.47	D
	ATOM	6209	ND2	ASN	D	332	120.165	19.468	23.815	1.00	52.34	D
	ATOM	6210	C	ASN	D	332	120.451	14.972	23.336	1.00	45.93	D
	ATOM	6211	O	ASN	D	332	120.420	14.681	22.140	1.00	45.54	D
5	ATOM	6212	N	SER	D	333	121.326	14.443	24.175	1.00	46.43	D
	ATOM	6213	CA	SER	D	333	122.308	13.487	23.702	1.00	45.98	D
	ATOM	6214	CB	SER	D	333	123.043	12.863	24.885	1.00	46.48	D
	ATOM	6215	OG	SER	D	333	123.853	11.783	24.454	1.00	49.00	D
	ATOM	6216	C	SER	D	333	121.659	12.392	22.851	1.00	44.33	D
10	ATOM	6217	O	SER	D	333	122.129	12.099	21.751	1.00	44.40	D
	ATOM	6218	N	LEU	D	334	120.577	11.795	23.344	1.00	42.68	D
	ATOM	6219	CA	LEU	D	334	119.912	10.728	22.591	1.00	41.52	D
	ATOM	6220	CB	LEU	D	334	118.777	10.098	23.407	1.00	39.72	D
	ATOM	6221	CG	LEU	D	334	117.873	9.152	22.604	1.00	38.51	D
15	ATOM	6222	CD1	LEU	D	334	118.687	7.997	22.053	1.00	37.25	D
	ATOM	6223	CD2	LEU	D	334	116.746	8.651	23.475	1.00	37.57	D
	ATOM	6224	C	LEU	D	334	119.352	11.228	21.268	1.00	39.88	D
	ATOM	6225	O	LEU	D	334	119.439	10.553	20.242	1.00	37.95	D
	ATOM	6226	N	ASN	D	335	118.758	12.410	21.304	1.00	39.39	D
20	ATOM	6227	CA	ASN	D	335	118.202	12.973	20.096	1.00	39.71	D
	ATOM	6228	CB	ASN	D	335	117.463	14.263	20.399	1.00	40.92	D
	ATOM	6229	CG	ASN	D	335	116.080	14.255	19.829	1.00	42.75	D
	ATOM	6230	OD1	ASN	D	335	115.879	13.877	18.676	1.00	43.99	D
	ATOM	6231	ND2	ASN	D	335	115.108	14.669	20.630	1.00	44.96	D
25	ATOM	6232	C	ASN	D	335	119.299	13.229	19.066	1.00	38.88	D
	ATOM	6233	O	ASN	D	335	119.209	12.772	17.926	1.00	39.28	D
	ATOM	6234	N	LEU	D	336	120.341	13.945	19.469	1.00	36.54	D
	ATOM	6235	CA	LEU	D	336	121.426	14.216	18.555	1.00	35.78	D
	ATOM	6236	CB	LEU	D	336	122.488	15.081	19.230	1.00	35.28	D
30	ATOM	6237	CG	LEU	D	336	123.704	15.571	18.421	1.00	35.06	D
	ATOM	6238	CD1	LEU	D	336	124.755	14.482	18.364	1.00	33.88	D
	ATOM	6239	CD2	LEU	D	336	123.284	16.002	17.027	1.00	33.93	D
	ATOM	6240	C	LEU	D	336	122.021	12.905	18.034	1.00	36.03	D
	ATOM	6241	O	LEU	D	336	122.542	12.857	16.920	1.00	37.69	D
35	ATOM	6242	N	LYS	D	337	121.919	11.833	18.812	1.00	36.19	D
	ATOM	6243	CA	LYS	D	337	122.439	10.529	18.378	1.00	37.20	D
	ATOM	6244	CB	LYS	D	337	122.452	9.533	19.547	1.00	38.40	D
	ATOM	6245	CG	LYS	D	337	123.706	9.512	20.409	1.00	40.10	D
	ATOM	6246	CD	LYS	D	337	124.743	8.543	19.848	1.00	41.01	D
40	ATOM	6247	CE	LYS	D	337	125.896	8.283	20.827	1.00	41.41	D
	ATOM	6248	NZ	LYS	D	337	125.504	7.528	22.071	1.00	40.33	D
	ATOM	6249	C	LYS	D	337	121.576	9.939	17.257	1.00	37.31	D
	ATOM	6250	O	LYS	D	337	122.081	9.279	16.344	1.00	37.48	D
	ATOM	6251	N	LEU	D	338	120.268	10.164	17.347	1.00	36.91	D
45	ATOM	6252	CA	LEU	D	338	119.332	9.654	16.351	1.00	36.87	D
	ATOM	6253	CB	LEU	D	338	117.893	9.797	16.863	1.00	35.09	D
	ATOM	6254	CG	LEU	D	338	117.529	8.902	18.052	1.00	33.33	D
	ATOM	6255	CD1	LEU	D	338	116.175	9.300	18.621	1.00	31.89	D
	ATOM	6256	CD2	LEU	D	338	117.533	7.450	17.600	1.00	31.70	D
50	ATOM	6257	C	LEU	D	338	119.513	10.412	15.044	1.00	37.22	D
	ATOM	6258	O	LEU	D	338	119.418	9.841	13.968	1.00	36.68	D
	ATOM	6259	N	SER	D	339	119.791	11.703	15.161	1.00	37.23	D
	ATOM	6260	CA	SER	D	339	120.000	12.537	14.006	1.00	35.92	D
	ATOM	6261	CB	SER	D	339	120.390	13.933	14.426	1.00	34.24	D

	ATOM	6262	OG	SER	D	339	120.457	14.756	13.283	1.00	37.68	D
	ATOM	6263	C	SER	D	339	121.094	11.973	13.124	1.00	36.83	D
	ATOM	6264	O	SER	D	339	120.978	12.005	11.908	1.00	36.94	D
	ATOM	6265	N	GLN	D	340	122.161	11.467	13.735	1.00	36.98	D
5	ATOM	6266	CA	GLN	D	340	123.266	10.895	12.975	1.00	37.54	D
	ATOM	6267	CB	GLN	D	340	124.443	10.581	13.883	1.00	38.76	D
	ATOM	6268	CG	GLN	D	340	124.489	11.408	15.144	1.00	42.76	D
	ATOM	6269	CD	GLN	D	340	125.519	12.491	15.095	1.00	43.21	D
	ATOM	6270	OE1	GLN	D	340	125.816	13.113	16.105	1.00	43.96	D
10	ATOM	6271	NE2	GLN	D	340	126.077	12.727	13.917	1.00	47.75	D
	ATOM	6272	C	GLN	D	340	122.786	9.592	12.376	1.00	38.02	D
	ATOM	6273	O	GLN	D	340	123.099	9.254	11.235	1.00	36.84	D
	ATOM	6274	N	LYS	D	341	122.023	8.857	13.172	1.00	38.91	D
	ATOM	6275	CA	LYS	D	341	121.503	7.564	12.759	1.00	40.04	D
15	ATOM	6276	CB	LYS	D	341	120.908	6.842	13.979	1.00	41.15	D
	ATOM	6277	CG	LYS	D	341	120.440	5.417	13.722	1.00	43.83	D
	ATOM	6278	CD	LYS	D	341	121.542	4.580	13.081	1.00	46.84	D
	ATOM	6279	CE	LYS	D	341	121.018	3.233	12.559	1.00	48.14	D
	ATOM	6280	NZ	LYS	D	341	122.101	2.428	11.901	1.00	48.02	D
20	ATOM	6281	C	LYS	D	341	120.463	7.656	11.641	1.00	40.03	D
	ATOM	6282	O	LYS	D	341	120.548	6.935	10.647	1.00	40.71	D
	ATOM	6283	N	TYR	D	342	119.494	8.551	11.804	1.00	39.52	D
	ATOM	6284	CA	TYR	D	342	118.413	8.726	10.840	1.00	39.22	D
	ATOM	6285	CB	TYR	D	342	117.084	8.349	11.504	1.00	40.25	D
25	ATOM	6286	CG	TYR	D	342	117.093	6.975	12.120	1.00	41.96	D
	ATOM	6287	CD1	TYR	D	342	117.151	5.839	11.322	1.00	44.58	D
	ATOM	6288	CE1	TYR	D	342	117.195	4.559	11.887	1.00	46.16	D
	ATOM	6289	CD2	TYR	D	342	117.076	6.805	13.501	1.00	43.49	D
	ATOM	6290	CE2	TYR	D	342	117.119	5.530	14.078	1.00	44.33	D
30	ATOM	6291	CZ	TYR	D	342	117.180	4.412	13.263	1.00	45.41	D
	ATOM	6292	OH	TYR	D	342	117.244	3.145	13.796	1.00	44.64	D
	ATOM	6293	C	TYR	D	342	118.315	10.155	10.287	1.00	38.30	D
	ATOM	6294	O	TYR	D	342	117.437	10.926	10.687	1.00	38.68	D
	ATOM	6295	N	PRO	D	343	119.207	10.522	9.354	1.00	36.69	D
35	ATOM	6296	CD	PRO	D	343	120.303	9.690	8.831	1.00	33.93	D
	ATOM	6297	CA	PRO	D	343	119.222	11.859	8.744	1.00	35.64	D
	ATOM	6298	CB	PRO	D	343	120.322	11.747	7.701	1.00	33.94	D
	ATOM	6299	CG	PRO	D	343	121.227	10.708	8.264	1.00	33.00	D
	ATOM	6300	C	PRO	D	343	117.897	12.243	8.100	1.00	36.66	D
40	ATOM	6301	O	PRO	D	343	117.387	13.353	8.298	1.00	36.68	D
	ATOM	6302	N	LYS	D	344	117.345	11.306	7.333	1.00	37.98	D
	ATOM	6303	CA	LYS	D	344	116.097	11.521	6.600	1.00	38.87	D
	ATOM	6304	CB	LYS	D	344	116.021	10.554	5.402	1.00	40.52	D
	ATOM	6305	CG	LYS	D	344	116.552	9.140	5.658	1.00	43.94	D
45	ATOM	6306	CD	LYS	D	344	115.598	8.274	6.494	1.00	44.39	D
	ATOM	6307	CE	LYS	D	344	116.370	7.166	7.227	1.00	43.37	D
	ATOM	6308	NZ	LYS	D	344	117.439	7.751	8.094	1.00	37.93	D
	ATOM	6309	C	LYS	D	344	114.791	11.471	7.396	1.00	37.24	D
	ATOM	6310	O	LYS	D	344	113.779	12.011	6.947	1.00	38.60	D
50	ATOM	6311	N	LEU	D	345	114.808	10.851	8.572	1.00	34.93	D
	ATOM	6312	CA	LEU	D	345	113.597	10.766	9.382	1.00	32.64	D
	ATOM	6313	CB	LEU	D	345	113.670	9.573	10.329	1.00	31.24	D
	ATOM	6314	CG	LEU	D	345	113.726	8.216	9.628	1.00	29.39	D
	ATOM	6315	CD1	LEU	D	345	113.660	7.118	10.667	1.00	30.86	D

	ATOM	6316	CD2	LEU	D	345	112.560	8.084	8.666	1.00	30.92	D
	ATOM	6317	C	LEU	D	345	113.376	12.033	10.176	1.00	31.59	D
	ATOM	6318	O	LEU	D	345	114.318	12.780	10.422	1.00	32.92	D
	ATOM	6319	N	SER	D	346	112.130	12.298	10.557	1.00	30.59	D
5	ATOM	6320	CA	SER	D	346	111.836	13.500	11.338	1.00	29.97	D
	ATOM	6321	CB	SER	D	346	110.377	13.931	11.158	1.00	29.48	D
	ATOM	6322	OG	SER	D	346	109.498	12.856	11.422	1.00	30.59	D
	ATOM	6323	C	SER	D	346	112.101	13.212	12.800	1.00	29.74	D
	ATOM	6324	O	SER	D	346	112.387	12.069	13.184	1.00	28.91	D
10	ATOM	6325	N	GLN	D	347	111.992	14.233	13.634	1.00	28.38	D
	ATOM	6326	CA	GLN	D	347	112.255	13.991	15.036	1.00	28.40	D
	ATOM	6327	CB	GLN	D	347	112.237	15.291	15.818	1.00	29.66	D
	ATOM	6328	CG	GLN	D	347	112.819	15.144	17.190	1.00	32.02	D
	ATOM	6329	CD	GLN	D	347	112.905	16.474	17.879	1.00	35.29	D
15	ATOM	6330	OE1	GLN	D	347	111.889	17.161	18.035	1.00	38.15	D
	ATOM	6331	NE2	GLN	D	347	114.111	16.861	18.292	1.00	33.64	D
	ATOM	6332	C	GLN	D	347	111.277	13.007	15.663	1.00	26.76	D
	ATOM	6333	O	GLN	D	347	111.694	12.085	16.357	1.00	26.57	D
	ATOM	6334	N	GLN	D	348	109.984	13.203	15.427	1.00	25.38	D
20	ATOM	6335	CA	GLN	D	348	108.996	12.306	16.001	1.00	24.96	D
	ATOM	6336	CB	GLN	D	348	107.581	12.739	15.657	1.00	24.21	D
	ATOM	6337	CG	GLN	D	348	107.267	14.152	16.034	1.00	24.28	D
	ATOM	6338	CD	GLN	D	348	107.648	15.126	14.947	1.00	23.84	D
	ATOM	6339	OE1	GLN	D	348	108.598	14.899	14.211	1.00	24.03	D
25	ATOM	6340	NE2	GLN	D	348	106.908	16.224	14.845	1.00	24.64	D
	ATOM	6341	C	GLN	D	348	109.209	10.896	15.483	1.00	26.54	D
	ATOM	6342	O	GLN	D	348	109.118	9.921	16.233	1.00	27.22	D
	ATOM	6343	N	ASP	D	349	109.499	10.791	14.193	1.00	26.70	D
	ATOM	6344	CA	ASP	D	349	109.718	9.500	13.588	1.00	26.16	D
30	ATOM	6345	CB	ASP	D	349	109.918	9.666	12.086	1.00	30.05	D
	ATOM	6346	CG	ASP	D	349	108.666	9.338	11.295	1.00	33.76	D
	ATOM	6347	OD1	ASP	D	349	107.598	9.889	11.612	1.00	35.36	D
	ATOM	6348	OD2	ASP	D	349	108.754	8.521	10.354	1.00	37.16	D
	ATOM	6349	C	ASP	D	349	110.900	8.775	14.220	1.00	25.17	D
35	ATOM	6350	O	ASP	D	349	110.815	7.578	14.508	1.00	25.67	D
	ATOM	6351	N	ARG	D	350	111.999	9.491	14.430	1.00	23.55	D
	ATOM	6352	CA	ARG	D	350	113.194	8.906	15.047	1.00	23.54	D
	ATOM	6353	CB	ARG	D	350	114.265	9.981	15.252	1.00	25.20	D
	ATOM	6354	CG	ARG	D	350	114.885	10.512	13.994	1.00	25.82	D
40	ATOM	6355	CD	ARG	D	350	115.595	11.837	14.220	1.00	25.92	D
	ATOM	6356	NE	ARG	D	350	116.255	12.230	12.977	1.00	28.94	D
	ATOM	6357	CZ	ARG	D	350	116.707	13.448	12.698	1.00	29.47	D
	ATOM	6358	NH1	ARG	D	350	116.590	14.440	13.568	1.00	32.83	D
	ATOM	6359	NH2	ARG	D	350	117.281	13.673	11.534	1.00	31.17	D
45	ATOM	6360	C	ARG	D	350	112.831	8.343	16.416	1.00	23.18	D
	ATOM	6361	O	ARG	D	350	112.968	7.148	16.679	1.00	22.24	D
	ATOM	6362	N	LEU	D	351	112.376	9.242	17.282	1.00	21.94	D
	ATOM	6363	CA	LEU	D	351	111.991	8.890	18.627	1.00	20.55	D
	ATOM	6364	CB	LEU	D	351	111.307	10.082	19.297	1.00	18.30	D
50	ATOM	6365	CG	LEU	D	351	112.227	11.278	19.543	1.00	15.70	D
	ATOM	6366	CD1	LEU	D	351	111.401	12.443	19.998	1.00	14.97	D
	ATOM	6367	CD2	LEU	D	351	113.315	10.927	20.561	1.00	12.36	D
	ATOM	6368	C	LEU	D	351	111.081	7.671	18.627	1.00	20.79	D
	ATOM	6369	O	LEU	D	351	111.175	6.824	19.508	1.00	21.85	D

	ATOM	6370	N	ARG	D	352	110.211	7.569	17.631	1.00	21.27	D
	ATOM	6371	CA	ARG	D	352	109.333	6.421	17.566	1.00	22.32	D
	ATOM	6372	CB	ARG	D	352	108.251	6.616	16.517	1.00	23.50	D
	ATOM	6373	CG	ARG	D	352	107.278	5.440	16.398	1.00	25.41	D
5	ATOM	6374	CD	ARG	D	352	106.075	5.874	15.568	1.00	26.94	D
	ATOM	6375	NE	ARG	D	352	106.491	6.312	14.248	1.00	27.67	D
	ATOM	6376	CZ	ARG	D	352	106.345	5.590	13.151	1.00	27.98	D
	ATOM	6377	NH1	ARG	D	352	105.772	4.384	13.223	1.00	28.77	D
	ATOM	6378	NH2	ARG	D	352	106.801	6.071	11.997	1.00	28.35	D
10	ATOM	6379	C	ARG	D	352	110.132	5.156	17.257	1.00	22.65	D
	ATOM	6380	O	ARG	D	352	109.852	4.088	17.809	1.00	22.75	D
	ATOM	6381	N	LEU	D	353	111.129	5.236	16.389	1.00	23.22	D
	ATOM	6382	CA	LEU	D	353	111.877	4.014	16.139	1.00	25.64	D
	ATOM	6383	CB	LEU	D	353	112.853	4.180	14.974	1.00	27.60	D
15	ATOM	6384	CG	LEU	D	353	112.211	4.675	13.687	1.00	31.53	D
	ATOM	6385	CD1	LEU	D	353	113.257	4.543	12.590	1.00	34.73	D
	ATOM	6386	CD2	LEU	D	353	110.948	3.847	13.321	1.00	34.02	D
	ATOM	6387	C	LEU	D	353	112.640	3.650	17.408	1.00	24.34	D
	ATOM	6388	O	LEU	D	353	112.766	2.477	17.748	1.00	24.26	D
20	ATOM	6389	N	SER	D	354	113.135	4.654	18.124	1.00	24.48	D
	ATOM	6390	CA	SER	D	354	113.888	4.379	19.339	1.00	24.64	D
	ATOM	6391	CB	SER	D	354	114.399	5.670	19.953	1.00	24.29	D
	ATOM	6392	OG	SER	D	354	115.774	5.509	20.223	1.00	27.22	D
	ATOM	6393	C	SER	D	354	113.045	3.623	20.345	1.00	23.77	D
25	ATOM	6394	O	SER	D	354	113.439	2.566	20.828	1.00	22.40	D
	ATOM	6395	N	PHE	D	355	111.879	4.169	20.646	1.00	23.57	D
	ATOM	6396	CA	PHE	D	355	110.979	3.533	21.573	1.00	25.63	D
	ATOM	6397	CB	PHE	D	355	109.660	4.283	21.596	1.00	26.61	D
	ATOM	6398	CG	PHE	D	355	108.725	3.795	22.636	1.00	27.78	D
30	ATOM	6399	CD1	PHE	D	355	109.055	3.919	23.978	1.00	29.88	D
	ATOM	6400	CD2	PHE	D	355	107.526	3.189	22.286	1.00	29.67	D
	ATOM	6401	CE1	PHE	D	355	108.205	3.443	24.972	1.00	29.34	D
	ATOM	6402	CE2	PHE	D	355	106.664	2.707	23.269	1.00	30.25	D
	ATOM	6403	CZ	PHE	D	355	107.011	2.836	24.614	1.00	29.64	D
35	ATOM	6404	C	PHE	D	355	110.731	2.089	21.156	1.00	26.53	D
	ATOM	6405	O	PHE	D	355	110.970	1.156	21.920	1.00	26.93	D
	ATOM	6406	N	LEU	D	356	110.257	1.904	19.931	1.00	27.97	D
	ATOM	6407	CA	LEU	D	356	109.975	0.557	19.441	1.00	29.40	D
	ATOM	6408	CB	LEU	D	356	109.502	0.601	17.990	1.00	29.41	D
40	ATOM	6409	CG	LEU	D	356	108.233	1.408	17.701	1.00	30.81	D
	ATOM	6410	CD1	LEU	D	356	108.091	1.510	16.193	1.00	30.03	D
	ATOM	6411	CD2	LEU	D	356	107.001	0.766	18.334	1.00	27.79	D
	ATOM	6412	C	LEU	D	356	111.164	-0.387	19.557	1.00	29.19	D
	ATOM	6413	O	LEU	D	356	111.011	-1.540	19.954	1.00	29.03	D
45	ATOM	6414	N	GLU	D	357	112.348	0.106	19.223	1.00	29.15	D
	ATOM	6415	CA	GLU	D	357	113.525	-0.723	19.296	1.00	30.63	D
	ATOM	6416	CB	GLU	D	357	114.677	-0.053	18.560	1.00	32.16	D
	ATOM	6417	CG	GLU	D	357	115.697	-1.025	18.007	1.00	37.30	D
	ATOM	6418	CD	GLU	D	357	117.086	-0.418	17.930	1.00	40.82	D
50	ATOM	6419	OE1	GLU	D	357	117.248	0.639	17.262	1.00	41.37	D
	ATOM	6420	OE2	GLU	D	357	118.017	-1.000	18.548	1.00	41.48	D
	ATOM	6421	C	GLU	D	357	113.946	-1.025	20.741	1.00	32.26	D
	ATOM	6422	O	GLU	D	357	114.599	-2.041	21.016	1.00	31.90	D
	ATOM	6423	N	ASN	D	358	113.571	-0.148	21.665	1.00	29.36	D

	ATOM	6424	CA	ASN	D	358	113.939	-0.341	23.046	1.00	27.42	D
	ATOM	6425	CB	ASN	D	358	114.060	1.000	23.750	1.00	27.90	D
	ATOM	6426	CG	ASN	D	358	115.443	1.598	23.610	1.00	28.81	D
	ATOM	6427	OD1	ASN	D	358	115.621	2.656	23.006	1.00	29.58	D
5	ATOM	6428	ND2	ASN	D	358	116.439	0.916	24.171	1.00	29.80	D
	ATOM	6429	C	ASN	D	358	112.996	-1.248	23.793	1.00	27.49	D
	ATOM	6430	O	ASN	D	358	113.404	-1.974	24.700	1.00	27.75	D
	ATOM	6431	N	ILE	D	359	111.732	-1.217	23.408	1.00	27.57	D
	ATOM	6432	CA	ILE	D	359	110.757	-2.076	24.046	1.00	28.89	D
10	ATOM	6433	CB	ILE	D	359	109.361	-1.821	23.510	1.00	29.72	D
	ATOM	6434	CG2	ILE	D	359	108.342	-2.575	24.322	1.00	28.76	D
	ATOM	6435	CG1	ILE	D	359	109.058	-0.336	23.581	1.00	32.82	D
	ATOM	6436	CD1	ILE	D	359	108.196	0.120	22.444	1.00	36.53	D
	ATOM	6437	C	ILE	D	359	111.161	-3.466	23.629	1.00	28.09	D
15	ATOM	6438	O	ILE	D	359	111.164	-4.389	24.425	1.00	27.60	D
	ATOM	6439	N	PHE	D	360	111.518	-3.592	22.361	1.00	29.39	D
	ATOM	6440	CA	PHE	D	360	111.926	-4.864	21.810	1.00	30.15	D
	ATOM	6441	CB	PHE	D	360	112.415	-4.654	20.372	1.00	32.47	D
	ATOM	6442	CG	PHE	D	360	112.998	-5.885	19.738	1.00	33.66	D
20	ATOM	6443	CD1	PHE	D	360	112.236	-7.045	19.600	1.00	34.21	D
	ATOM	6444	CD2	PHE	D	360	114.327	-5.898	19.326	1.00	34.66	D
	ATOM	6445	CE1	PHE	D	360	112.790	-8.201	19.071	1.00	34.86	D
	ATOM	6446	CE2	PHE	D	360	114.894	-7.044	18.796	1.00	36.23	D
	ATOM	6447	CZ	PHE	D	360	114.124	-8.202	18.670	1.00	35.77	D
25	ATOM	6448	C	PHE	D	360	113.015	-5.503	22.654	1.00	29.32	D
	ATOM	6449	O	PHE	D	360	112.879	-6.641	23.092	1.00	29.82	D
	ATOM	6450	N	ILE	D	361	114.093	-4.762	22.880	1.00	28.24	D
	ATOM	6451	CA	ILE	D	361	115.222	-5.254	23.660	1.00	26.57	D
	ATOM	6452	CB	ILE	D	361	116.376	-4.219	23.597	1.00	26.56	D
30	ATOM	6453	CG2	ILE	D	361	117.540	-4.638	24.502	1.00	24.26	D
	ATOM	6454	CG1	ILE	D	361	116.855	-4.117	22.140	1.00	25.22	D
	ATOM	6455	CD1	ILE	D	361	117.841	-3.000	21.868	1.00	25.88	D
	ATOM	6456	C	ILE	D	361	114.834	-5.578	25.111	1.00	25.14	D
	ATOM	6457	O	ILE	D	361	115.238	-6.610	25.656	1.00	24.17	D
35	ATOM	6458	N	LEU	D	362	114.027	-4.712	25.718	1.00	22.80	D
	ATOM	6459	CA	LEU	D	362	113.591	-4.915	27.098	1.00	23.19	D
	ATOM	6460	CB	LEU	D	362	112.801	-3.700	27.576	1.00	20.92	D
	ATOM	6461	CG	LEU	D	362	112.565	-3.604	29.077	1.00	20.66	D
	ATOM	6462	CD1	LEU	D	362	113.860	-3.753	29.867	1.00	18.78	D
40	ATOM	6463	CD2	LEU	D	362	111.917	-2.273	29.338	1.00	20.71	D
	ATOM	6464	C	LEU	D	362	112.773	-6.196	27.330	1.00	23.63	D
	ATOM	6465	O	LEU	D	362	112.997	-6.915	28.311	1.00	23.67	D
	ATOM	6466	N	LYS	D	363	111.824	-6.453	26.434	1.00	23.53	D
	ATOM	6467	CA	LYS	D	363	110.986	-7.639	26.477	1.00	24.42	D
45	ATOM	6468	CB	LYS	D	363	110.156	-7.743	25.191	1.00	26.43	D
	ATOM	6469	CG	LYS	D	363	108.730	-7.209	25.270	1.00	30.86	D
	ATOM	6470	CD	LYS	D	363	108.669	-5.840	25.929	1.00	33.41	D
	ATOM	6471	CE	LYS	D	363	107.226	-5.421	26.252	1.00	35.72	D
	ATOM	6472	NZ	LYS	D	363	107.204	-4.294	27.264	1.00	35.50	D
50	ATOM	6473	C	LYS	D	363	111.901	-8.859	26.573	1.00	25.36	D
	ATOM	6474	O	LYS	D	363	111.629	-9.802	27.311	1.00	25.60	D
	ATOM	6475	N	ASN	D	364	112.988	-8.829	25.809	1.00	25.23	D
	ATOM	6476	CA	ASN	D	364	113.935	-9.927	25.799	1.00	25.39	D
	ATOM	6477	CB	ASN	D	364	114.980	-9.737	24.712	1.00	25.02	D

	ATOM	6478	CG	ASN	D	364	114.436	-9.985	23.348	1.00	26.12	D
	ATOM	6479	OD1	ASN	D	364	115.038	-9.589	22.348	1.00	25.32	D
	ATOM	6480	ND2	ASN	D	364	113.286	-10.662	23.283	1.00	27.95	D
	ATOM	6481	C	ASN	D	364	114.640	-10.030	27.118	1.00	26.63	D
5	ATOM	6482	O	ASN	D	364	114.785	-11.120	27.665	1.00	28.76	D
	ATOM	6483	N	TRP	D	365	115.101	-8.901	27.635	1.00	26.04	D
	ATOM	6484	CA	TRP	D	365	115.794	-8.937	28.906	1.00	25.62	D
	ATOM	6485	CB	TRP	D	365	116.211	-7.535	29.357	1.00	23.36	D
	ATOM	6486	CG	TRP	D	365	117.514	-7.035	28.789	1.00	19.48	D
10	ATOM	6487	CD2	TRP	D	365	118.801	-7.069	29.427	1.00	16.99	D
	ATOM	6488	CE2	TRP	D	365	119.706	-6.410	28.572	1.00	15.60	D
	ATOM	6489	CE3	TRP	D	365	119.275	-7.589	30.640	1.00	15.17	D
	ATOM	6490	CD1	TRP	D	365	117.691	-6.387	27.613	1.00	17.39	D
	ATOM	6491	NE1	TRP	D	365	119.001	-6.003	27.473	1.00	14.98	D
15	ATOM	6492	CZ2	TRP	D	365	121.072	-6.249	28.892	1.00	15.36	D
	ATOM	6493	CZ3	TRP	D	365	120.628	-7.428	30.956	1.00	13.84	D
	ATOM	6494	CH2	TRP	D	365	121.509	-6.762	30.081	1.00	10.82	D
	ATOM	6495	C	TRP	D	365	114.868	-9.538	29.947	1.00	26.26	D
	ATOM	6496	O	TRP	D	365	115.267	-10.422	30.693	1.00	28.48	D
20	ATOM	6497	N	TYR	D	366	113.621	-9.084	29.956	1.00	24.80	D
	ATOM	6498	CA	TYR	D	366	112.641	-9.530	30.934	1.00	23.32	D
	ATOM	6499	CB	TYR	D	366	111.480	-8.553	30.947	1.00	17.63	D
	ATOM	6500	CG	TYR	D	366	111.793	-7.211	31.597	1.00	16.02	D
	ATOM	6501	CD1	TYR	D	366	113.058	-6.914	32.118	1.00	14.32	D
25	ATOM	6502	CE1	TYR	D	366	113.304	-5.681	32.726	1.00	11.48	D
	ATOM	6503	CD2	TYR	D	366	110.808	-6.243	31.712	1.00	13.79	D
	ATOM	6504	CE2	TYR	D	366	111.054	-5.033	32.320	1.00	11.61	D
	ATOM	6505	CZ	TYR	D	366	112.283	-4.760	32.812	1.00	11.97	D
	ATOM	6506	OH	TYR	D	366	112.475	-3.532	33.364	1.00	15.79	D
30	ATOM	6507	C	TYR	D	366	112.112	-10.939	30.762	1.00	25.30	D
	ATOM	6508	O	TYR	D	366	111.620	-11.548	31.715	1.00	25.60	D
	ATOM	6509	N	ASN	D	367	112.227	-11.441	29.538	1.00	27.79	D
	ATOM	6510	CA	ASN	D	367	111.757	-12.770	29.160	1.00	28.52	D
	ATOM	6511	CB	ASN	D	367	111.596	-12.837	27.642	1.00	29.23	D
35	ATOM	6512	CG	ASN	D	367	111.047	-14.162	27.168	1.00	29.51	D
	ATOM	6513	OD1	ASN	D	367	111.045	-15.165	27.907	1.00	29.16	D
	ATOM	6514	ND2	ASN	D	367	110.588	-14.183	25.915	1.00	28.51	D
	ATOM	6515	C	ASN	D	367	112.706	-13.872	29.617	1.00	28.04	D
	ATOM	6516	O	ASN	D	367	113.779	-14.076	29.042	1.00	28.99	D
40	ATOM	6517	N	PRO	D	368	112.306	-14.606	30.659	1.00	27.46	D
	ATOM	6518	CD	PRO	D	368	111.038	-14.427	31.394	1.00	27.49	D
	ATOM	6519	CA	PRO	D	368	113.094	-15.701	31.228	1.00	26.35	D
	ATOM	6520	CB	PRO	D	368	112.174	-16.249	32.313	1.00	26.40	D
	ATOM	6521	CG	PRO	D	368	111.350	-15.041	32.703	1.00	26.24	D
45	ATOM	6522	C	PRO	D	368	113.470	-16.766	30.207	1.00	25.90	D
	ATOM	6523	O	PRO	D	368	114.556	-17.338	30.270	1.00	23.69	D
	ATOM	6524	N	LYS	D	369	112.570	-17.027	29.264	1.00	26.98	D
	ATOM	6525	CA	LYS	D	369	112.815	-18.051	28.249	1.00	27.69	D
	ATOM	6526	CB	LYS	D	369	111.483	-18.478	27.605	1.00	27.37	D
50	ATOM	6527	CG	LYS	D	369	111.523	-19.857	26.933	1.00	28.34	D
	ATOM	6528	CD	LYS	D	369	110.159	-20.280	26.431	0.00	28.71	D
	ATOM	6529	CE	LYS	D	369	109.692	-19.395	25.288	0.00	29.07	D
	ATOM	6530	NZ	LYS	D	369	108.385	-19.851	24.737	0.00	29.21	D
	ATOM	6531	C	LYS	D	369	113.815	-17.602	27.170	1.00	28.21	D

	ATOM	6532	O	LYS	D	369	114.404	-18.432	26.466	1.00	27.80	D
	ATOM	6533	N	PHE	D	370	114.027	-16.295	27.055	1.00	28.20	D
	ATOM	6534	CA	PHE	D	370	114.945	-15.779	26.048	1.00	29.53	D
	ATOM	6535	CB	PHE	D	370	114.804	-14.267	25.930	1.00	30.24	D
5	ATOM	6536	CG	PHE	D	370	115.741	-13.647	24.926	1.00	31.46	D
	ATOM	6537	CD1	PHE	D	370	117.107	-13.497	25.208	1.00	32.17	D
	ATOM	6538	CD2	PHE	D	370	115.253	-13.184	23.711	1.00	31.98	D
	ATOM	6539	CE1	PHE	D	370	117.970	-12.894	24.301	1.00	30.34	D
	ATOM	6540	CE2	PHE	D	370	116.105	-12.580	22.795	1.00	32.40	D
10	ATOM	6541	CZ	PHE	D	370	117.473	-12.434	23.098	1.00	31.69	D
	ATOM	6542	C	PHE	D	370	116.418	-16.125	26.250	1.00	29.47	D
	ATOM	6543	O	PHE	D	370	116.990	-15.909	27.323	1.00	30.76	D
	ATOM	6544	N	VAL	D	371	117.038	-16.623	25.186	1.00	28.02	D
	ATOM	6545	CA	VAL	D	371	118.441	-16.986	25.252	1.00	27.30	D
15	ATOM	6546	CB	VAL	D	371	118.648	-18.446	24.756	1.00	26.04	D
	ATOM	6547	CG1	VAL	D	371	120.104	-18.829	24.825	1.00	22.81	D
	ATOM	6548	CG2	VAL	D	371	117.827	-19.396	25.624	1.00	22.71	D
	ATOM	6549	C	VAL	D	371	119.309	-15.995	24.469	1.00	28.27	D
	ATOM	6550	O	VAL	D	371	119.221	-15.880	23.248	1.00	27.93	D
20	ATOM	6551	N	PRO	D	372	120.161	-15.251	25.188	1.00	29.70	D
	ATOM	6552	CD	PRO	D	372	120.326	-15.276	26.648	1.00	29.18	D
	ATOM	6553	CA	PRO	D	372	121.057	-14.258	24.597	1.00	31.17	D
	ATOM	6554	CB	PRO	D	372	121.744	-13.642	25.816	1.00	29.97	D
	ATOM	6555	CG	PRO	D	372	120.796	-13.886	26.914	1.00	30.31	D
25	ATOM	6556	C	PRO	D	372	122.071	-14.884	23.659	1.00	32.23	D
	ATOM	6557	O	PRO	D	372	122.136	-16.104	23.515	1.00	33.92	D
	ATOM	6558	N	GLN	D	373	122.860	-14.033	23.019	1.00	32.64	D
	ATOM	6559	CA	GLN	D	373	123.907	-14.511	22.144	1.00	31.91	D
	ATOM	6560	CB	GLN	D	373	123.945	-13.701	20.865	1.00	31.03	D
30	ATOM	6561	CG	GLN	D	373	124.881	-14.279	19.845	1.00	31.69	D
	ATOM	6562	CD	GLN	D	373	125.575	-13.202	19.069	1.00	32.49	D
	ATOM	6563	OE1	GLN	D	373	124.937	-12.328	18.502	1.00	33.06	D
	ATOM	6564	NE2	GLN	D	373	126.892	-13.251	19.045	1.00	34.46	D
	ATOM	6565	C	GLN	D	373	125.203	-14.315	22.925	1.00	31.35	D
35	ATOM	6566	O	GLN	D	373	125.612	-13.192	23.224	1.00	31.52	D
	ATOM	6567	N	ARG	D	374	125.842	-15.418	23.264	1.00	29.71	D
	ATOM	6568	CA	ARG	D	374	127.059	-15.342	24.024	1.00	29.87	D
	ATOM	6569	CB	ARG	D	374	127.054	-16.417	25.102	1.00	30.39	D
	ATOM	6570	CG	ARG	D	374	128.347	-16.511	25.854	1.00	31.03	D
40	ATOM	6571	CD	ARG	D	374	128.261	-17.597	26.873	1.00	31.27	D
	ATOM	6572	NE	ARG	D	374	129.475	-17.599	27.658	1.00	32.88	D
	ATOM	6573	CZ	ARG	D	374	129.738	-18.450	28.637	1.00	33.11	D
	ATOM	6574	NH1	ARG	D	374	128.856	-19.390	28.956	1.00	31.68	D
	ATOM	6575	NH2	ARG	D	374	130.889	-18.343	29.301	1.00	33.83	D
45	ATOM	6576	C	ARG	D	374	128.306	-15.477	23.161	1.00	30.20	D
	ATOM	6577	O	ARG	D	374	128.383	-16.319	22.268	1.00	30.52	D
	ATOM	6578	N	THR	D	375	129.298	-14.654	23.463	1.00	30.06	D
	ATOM	6579	CA	THR	D	375	130.543	-14.641	22.724	1.00	29.07	D
	ATOM	6580	CB	THR	D	375	130.574	-13.423	21.801	1.00	29.18	D
50	ATOM	6581	OG1	THR	D	375	129.254	-13.177	21.294	1.00	30.22	D
	ATOM	6582	CG2	THR	D	375	131.520	-13.650	20.650	1.00	27.55	D
	ATOM	6583	C	THR	D	375	131.666	-14.506	23.749	1.00	29.99	D
	ATOM	6584	O	THR	D	375	131.743	-13.505	24.473	1.00	30.81	D
	ATOM	6585	N	THR	D	376	132.537	-15.504	23.824	1.00	29.02	D

	ATOM	6586	CA	THR	D	376	133.631	-15.459	24.789	1.00	28.35	D
	ATOM	6587	CB	THR	D	376	133.775	-16.810	25.551	1.00	26.89	D
	ATOM	6588	OG1	THR	D	376	132.516	-17.174	26.129	1.00	24.67	D
	ATOM	6589	CG2	THR	D	376	134.822	-16.700	26.648	1.00	25.06	D
5	ATOM	6590	C	THR	D	376	134.959	-15.155	24.120	1.00	29.32	D
	ATOM	6591	O	THR	D	376	135.386	-15.886	23.234	1.00	28.86	D
	ATOM	6592	N	LEU	D	377	135.616	-14.081	24.555	1.00	31.19	D
	ATOM	6593	CA	LEU	D	377	136.916	-13.701	24.001	1.00	33.04	D
	ATOM	6594	CB	LEU	D	377	136.888	-12.242	23.558	1.00	31.62	D
10	ATOM	6595	CG	LEU	D	377	135.621	-11.843	22.793	1.00	32.74	D
	ATOM	6596	CD1	LEU	D	377	135.718	-10.396	22.376	1.00	32.01	D
	ATOM	6597	CD2	LEU	D	377	135.430	-12.735	21.590	1.00	32.02	D
	ATOM	6598	C	LEU	D	377	138.006	-13.907	25.044	1.00	35.05	D
	ATOM	6599	O	LEU	D	377	137.733	-13.877	26.241	1.00	36.55	D
15	ATOM	6600	N	ARG	D	378	139.238	-14.122	24.590	1.00	37.30	D
	ATOM	6601	CA	ARG	D	378	140.381	-14.341	25.487	1.00	38.75	D
	ATOM	6602	CB	ARG	D	378	141.620	-14.732	24.661	1.00	41.44	D
	ATOM	6603	CG	ARG	D	378	142.735	-15.467	25.412	1.00	45.29	D
	ATOM	6604	CD	ARG	D	378	143.962	-15.705	24.499	1.00	49.27	D
20	ATOM	6605	NE	ARG	D	378	144.615	-14.445	24.116	1.00	53.86	D
	ATOM	6606	CZ	ARG	D	378	145.636	-14.322	23.260	1.00	55.92	D
	ATOM	6607	NH1	ARG	D	378	146.147	-15.400	22.666	1.00	55.78	D
	ATOM	6608	NH2	ARG	D	378	146.152	-13.109	23.009	1.00	55.08	D
	ATOM	6609	C	ARG	D	378	140.663	-13.056	26.259	1.00	38.43	D
25	ATOM	6610	O	ARG	D	378	140.498	-11.956	25.723	1.00	37.88	D
	ATOM	6611	N	GLY	D	379	141.098	-13.206	27.510	1.00	38.54	D
	ATOM	6612	CA	GLY	D	379	141.408	-12.058	28.349	1.00	38.37	D
	ATOM	6613	C	GLY	D	379	142.901	-11.817	28.563	1.00	38.46	D
	ATOM	6614	O	GLY	D	379	143.704	-12.014	27.646	1.00	39.93	D
30	ATOM	6615	N	HIS	D	380	143.270	-11.390	29.771	1.00	36.54	D
	ATOM	6616	CA	HIS	D	380	144.663	-11.116	30.118	1.00	35.40	D
	ATOM	6617	CB	HIS	D	380	144.735	-10.098	31.259	1.00	32.54	D
	ATOM	6618	CG	HIS	D	380	144.169	-8.762	30.910	1.00	29.64	D
	ATOM	6619	CD2	HIS	D	380	144.748	-7.541	30.837	1.00	29.11	D
35	ATOM	6620	ND1	HIS	D	380	142.845	-8.580	30.581	1.00	28.66	D
	ATOM	6621	CE1	HIS	D	380	142.630	-7.302	30.323	1.00	26.84	D
	ATOM	6622	NE2	HIS	D	380	143.768	-6.650	30.470	1.00	28.50	D
	ATOM	6623	C	HIS	D	380	145.400	-12.389	30.524	1.00	35.86	D
	ATOM	6624	O	HIS	D	380	144.796	-13.450	30.606	1.00	35.08	D
40	ATOM	6625	N	MSE	D	381	146.699	-12.287	30.790	1.00	37.57	D
	ATOM	6626	CA	MSE	D	381	147.467	-13.465	31.172	1.00	40.68	D
	ATOM	6627	CB	MSE	D	381	148.937	-13.253	30.850	1.00	42.82	D
	ATOM	6628	CG	MSE	D	381	149.177	-13.111	29.372	1.00	45.44	D
	ATOM	6629	SE	MSE	D	381	150.909	-12.445	28.929	1.00	55.08	D
45	ATOM	6630	CE	MSE	D	381	150.582	-10.533	29.001	1.00	48.67	D
	ATOM	6631	C	MSE	D	381	147.306	-13.812	32.645	1.00	41.59	D
	ATOM	6632	O	MSE	D	381	147.979	-14.701	33.169	1.00	40.94	D
	ATOM	6633	N	THR	D	382	146.392	-13.103	33.296	1.00	42.55	D
	ATOM	6634	CA	THR	D	382	146.091	-13.286	34.704	1.00	42.91	D
50	ATOM	6635	CB	THR	D	382	146.571	-12.035	35.487	1.00	42.87	D
	ATOM	6636	OG1	THR	D	382	146.096	-12.083	36.838	1.00	47.41	D
	ATOM	6637	CG2	THR	D	382	146.091	-10.770	34.806	1.00	42.47	D
	ATOM	6638	C	THR	D	382	144.566	-13.490	34.809	1.00	42.80	D
	ATOM	6639	O	THR	D	382	143.799	-12.695	34.280	1.00	45.02	D

	ATOM	6640	N	SER	D	383	144.129	-14.559	35.466	1.00	41.05	D
	ATOM	6641	CA	SER	D	383	142.708	-14.855	35.590	1.00	40.03	D
	ATOM	6642	CB	SER	D	383	142.527	-16.201	36.285	1.00	41.63	D
	ATOM	6643	OG	SER	D	383	143.273	-16.252	37.491	1.00	42.67	D
5	ATOM	6644	C	SER	D	383	141.888	-13.806	36.323	1.00	38.85	D
	ATOM	6645	O	SER	D	383	140.701	-14.007	36.569	1.00	39.35	D
	ATOM	6646	N	VAL	D	384	142.514	-12.689	36.665	1.00	37.95	D
	ATOM	6647	CA	VAL	D	384	141.829	-11.620	37.382	1.00	37.40	D
	ATOM	6648	CB	VAL	D	384	142.471	-11.414	38.777	1.00	39.34	D
10	ATOM	6649	CG1	VAL	D	384	141.606	-10.515	39.638	1.00	39.21	D
	ATOM	6650	CG2	VAL	D	384	142.672	-12.756	39.451	1.00	41.87	D
	ATOM	6651	C	VAL	D	384	141.899	-10.302	36.615	1.00	35.77	D
	ATOM	6652	O	VAL	D	384	142.987	-9.824	36.282	1.00	35.80	D
	ATOM	6653	N	ILE	D	385	140.741	-9.719	36.330	1.00	33.56	D
15	ATOM	6654	CA	ILE	D	385	140.697	-8.445	35.627	1.00	31.75	D
	ATOM	6655	CB	ILE	D	385	139.503	-8.347	34.670	1.00	32.21	D
	ATOM	6656	CG2	ILE	D	385	139.566	-7.028	33.924	1.00	31.42	D
	ATOM	6657	CG1	ILE	D	385	139.528	-9.506	33.673	1.00	34.12	D
	ATOM	6658	CD1	ILE	D	385	140.728	-9.519	32.787	1.00	31.79	D
20	ATOM	6659	C	ILE	D	385	140.524	-7.369	36.681	1.00	29.87	D
	ATOM	6660	O	ILE	D	385	139.636	-7.468	37.523	1.00	29.33	D
	ATOM	6661	N	THR	D	386	141.364	-6.341	36.631	1.00	28.00	D
	ATOM	6662	CA	THR	D	386	141.284	-5.262	37.603	1.00	26.59	D
	ATOM	6663	CB	THR	D	386	142.665	-4.709	37.933	1.00	28.33	D
25	ATOM	6664	OG1	THR	D	386	143.147	-3.965	36.810	1.00	33.14	D
	ATOM	6665	CG2	THR	D	386	143.629	-5.847	38.258	1.00	27.95	D
	ATOM	6666	C	THR	D	386	140.370	-4.095	37.219	1.00	23.96	D
	ATOM	6667	O	THR	D	386	140.049	-3.258	38.057	1.00	23.82	D
	ATOM	6668	N	CYS	D	387	139.969	-4.000	35.959	1.00	21.99	D
30	ATOM	6669	CA	CYS	D	387	139.032	-2.946	35.583	1.00	21.32	D
	ATOM	6670	CB	CYS	D	387	139.593	-1.554	35.810	1.00	21.52	D
	ATOM	6671	SG	CYS	D	387	141.286	-1.370	35.494	1.00	24.48	D
	ATOM	6672	C	CYS	D	387	138.522	-3.058	34.185	1.00	20.32	D
	ATOM	6673	O	CYS	D	387	139.180	-3.609	33.309	1.00	20.62	D
35	ATOM	6674	N	LEU	D	388	137.313	-2.554	33.993	1.00	21.13	D
	ATOM	6675	CA	LEU	D	388	136.666	-2.620	32.699	1.00	21.99	D
	ATOM	6676	CB	LEU	D	388	135.720	-3.811	32.699	1.00	19.44	D
	ATOM	6677	CG	LEU	D	388	134.666	-3.896	31.603	1.00	17.83	D
	ATOM	6678	CD1	LEU	D	388	134.369	-5.364	31.382	1.00	19.58	D
40	ATOM	6679	CD2	LEU	D	388	133.406	-3.172	32.009	1.00	17.27	D
	ATOM	6680	C	LEU	D	388	135.910	-1.349	32.307	1.00	23.54	D
	ATOM	6681	O	LEU	D	388	135.262	-0.724	33.136	1.00	24.86	D
	ATOM	6682	N	GLN	D	389	136.011	-0.965	31.038	1.00	25.33	D
	ATOM	6683	CA	GLN	D	389	135.302	0.203	30.521	1.00	25.28	D
45	ATOM	6684	CB	GLN	D	389	136.275	1.296	30.073	1.00	25.97	D
	ATOM	6685	CG	GLN	D	389	137.029	2.071	31.150	1.00	25.10	D
	ATOM	6686	CD	GLN	D	389	136.179	3.114	31.877	1.00	26.41	D
	ATOM	6687	OE1	GLN	D	389	135.673	2.850	32.949	1.00	26.25	D
	ATOM	6688	NE2	GLN	D	389	136.031	4.304	31.293	1.00	27.94	D
50	ATOM	6689	C	GLN	D	389	134.477	-0.233	29.303	1.00	26.25	D
	ATOM	6690	O	GLN	D	389	134.917	-1.076	28.515	1.00	26.39	D
	ATOM	6691	N	PHE	D	390	133.284	0.340	29.153	1.00	27.94	D
	ATOM	6692	CA	PHE	D	390	132.415	0.045	28.015	1.00	28.91	D
	ATOM	6693	CB	PHE	D	390	131.364	-0.995	28.424	1.00	26.05	D

	ATOM	6694	CG	PHE	D	390	130.416	-1.381	27.322	1.00	26.58	D
	ATOM	6695	CD1	PHE	D	390	130.826	-1.411	25.998	1.00	27.31	D
	ATOM	6696	CD2	PHE	D	390	129.087	-1.675	27.609	1.00	27.25	D
	ATOM	6697	CE1	PHE	D	390	129.921	-1.716	24.978	1.00	26.45	D
5	ATOM	6698	CE2	PHE	D	390	128.179	-1.982	26.595	1.00	26.66	D
	ATOM	6699	CZ	PHE	D	390	128.597	-1.999	25.284	1.00	25.88	D
	ATOM	6700	C	PHE	D	390	131.800	1.375	27.521	1.00	31.17	D
	ATOM	6701	O	PHE	D	390	130.844	1.911	28.095	1.00	31.73	D
	ATOM	6702	N	GLU	D	391	132.404	1.908	26.460	1.00	33.23	D
10	ATOM	6703	CA	GLU	D	391	132.004	3.172	25.842	1.00	36.52	D
	ATOM	6704	CB	GLU	D	391	132.752	4.335	26.494	1.00	37.25	D
	ATOM	6705	CG	GLU	D	391	131.870	5.425	27.041	1.00	38.77	D
	ATOM	6706	CD	GLU	D	391	131.258	5.032	28.354	1.00	39.09	D
	ATOM	6707	OE1	GLU	D	391	132.023	4.888	29.322	1.00	40.49	D
15	ATOM	6708	OE2	GLU	D	391	130.024	4.859	28.417	1.00	39.48	D
	ATOM	6709	C	GLU	D	391	132.377	3.150	24.360	1.00	37.92	D
	ATOM	6710	O	GLU	D	391	133.293	2.426	23.956	1.00	39.21	D
	ATOM	6711	N	ASP	D	392	131.704	3.971	23.557	1.00	38.58	D
	ATOM	6712	CA	ASP	D	392	131.986	4.053	22.112	1.00	38.07	D
20	ATOM	6713	CB	ASP	D	392	133.157	5.009	21.858	1.00	37.43	D
	ATOM	6714	CG	ASP	D	392	132.716	6.428	21.778	1.00	39.32	D
	ATOM	6715	OD1	ASP	D	392	131.501	6.650	21.954	1.00	40.76	D
	ATOM	6716	OD2	ASP	D	392	133.557	7.317	21.530	1.00	40.53	D
	ATOM	6717	C	ASP	D	392	132.253	2.725	21.400	1.00	36.82	D
25	ATOM	6718	O	ASP	D	392	133.221	2.589	20.647	1.00	36.96	D
	ATOM	6719	N	ASN	D	393	131.381	1.753	21.631	1.00	35.81	D
	ATOM	6720	CA	ASN	D	393	131.513	0.448	21.000	1.00	36.51	D
	ATOM	6721	CB	ASN	D	393	131.410	0.572	19.471	1.00	37.62	D
	ATOM	6722	CG	ASN	D	393	130.111	1.264	19.001	1.00	39.78	D
30	ATOM	6723	OD1	ASN	D	393	130.023	1.696	17.846	1.00	41.53	D
	ATOM	6724	ND2	ASN	D	393	129.111	1.362	19.881	1.00	38.28	D
	ATOM	6725	C	ASN	D	393	132.829	-0.215	21.366	1.00	34.65	D
	ATOM	6726	O	ASN	D	393	133.249	-1.163	20.710	1.00	34.87	D
	ATOM	6727	N	TYR	D	394	133.477	0.292	22.409	1.00	33.42	D
35	ATOM	6728	CA	TYR	D	394	134.742	-0.264	22.884	1.00	32.37	D
	ATOM	6729	CB	TYR	D	394	135.783	0.838	23.102	1.00	32.07	D
	ATOM	6730	CG	TYR	D	394	136.458	1.349	21.860	1.00	32.95	D
	ATOM	6731	CD1	TYR	D	394	137.124	0.479	20.992	1.00	32.58	D
	ATOM	6732	CE1	TYR	D	394	137.777	0.953	19.858	1.00	31.50	D
40	ATOM	6733	CD2	TYR	D	394	136.459	2.704	21.565	1.00	31.89	D
	ATOM	6734	CE2	TYR	D	394	137.104	3.189	20.445	1.00	33.06	D
	ATOM	6735	CZ	TYR	D	394	137.762	2.316	19.594	1.00	33.32	D
	ATOM	6736	OH	TYR	D	394	138.406	2.827	18.492	1.00	33.69	D
	ATOM	6737	C	TYR	D	394	134.554	-0.956	24.224	1.00	32.16	D
45	ATOM	6738	O	TYR	D	394	133.692	-0.582	25.016	1.00	33.01	D
	ATOM	6739	N	VAL	D	395	135.359	-1.970	24.481	1.00	31.18	D
	ATOM	6740	CA	VAL	D	395	135.307	-2.636	25.767	1.00	30.34	D
	ATOM	6741	CB	VAL	D	395	134.724	-4.036	25.689	1.00	32.30	D
	ATOM	6742	CG1	VAL	D	395	134.537	-4.571	27.092	1.00	30.09	D
50	ATOM	6743	CG2	VAL	D	395	133.388	-4.017	24.945	1.00	32.97	D
	ATOM	6744	C	VAL	D	395	136.751	-2.752	26.150	1.00	29.50	D
	ATOM	6745	O	VAL	D	395	137.469	-3.592	25.608	1.00	30.47	D
	ATOM	6746	N	ILE	D	396	137.190	-1.895	27.061	1.00	27.33	D
	ATOM	6747	CA	ILE	D	396	138.579	-1.929	27.471	1.00	24.79	D

	ATOM	6748	CB	ILE	D	396	139.202	-0.529	27.477	1.00	20.54	D
	ATOM	6749	CG2	ILE	D	396	140.724	-0.654	27.607	1.00	18.18	D
	ATOM	6750	CG1	ILE	D	396	138.779	0.231	26.222	1.00	19.10	D
	ATOM	6751	CD1	ILE	D	396	137.698	1.261	26.480	1.00	15.50	D
5	ATOM	6752	C	ILE	D	396	138.721	-2.532	28.860	1.00	25.91	D
	ATOM	6753	O	ILE	D	396	137.839	-2.371	29.709	1.00	25.28	D
	ATOM	6754	N	THR	D	397	139.839	-3.228	29.075	1.00	25.38	D
	ATOM	6755	CA	THR	D	397	140.133	-3.867	30.352	1.00	24.35	D
	ATOM	6756	CB	THR	D	397	139.734	-5.353	30.367	1.00	23.41	D
10	ATOM	6757	OG1	THR	D	397	140.542	-6.067	29.425	1.00	22.79	D
	ATOM	6758	CG2	THR	D	397	138.280	-5.530	30.010	1.00	22.25	D
	ATOM	6759	C	THR	D	397	141.610	-3.834	30.732	1.00	25.66	D
	ATOM	6760	O	THR	D	397	142.492	-3.945	29.876	1.00	25.23	D
	ATOM	6761	N	GLY	D	398	141.871	-3.715	32.032	1.00	26.89	D
15	ATOM	6762	CA	GLY	D	398	143.239	-3.717	32.535	1.00	27.00	D
	ATOM	6763	C	GLY	D	398	143.440	-4.892	33.487	1.00	26.90	D
	ATOM	6764	O	GLY	D	398	142.464	-5.481	33.951	1.00	26.42	D
	ATOM	6765	N	ALA	D	399	144.692	-5.250	33.776	1.00	28.42	D
	ATOM	6766	CA	ALA	D	399	144.977	-6.367	34.694	1.00	29.91	D
20	ATOM	6767	CB	ALA	D	399	144.889	-7.701	33.945	1.00	28.40	D
	ATOM	6768	C	ALA	D	399	146.335	-6.265	35.410	1.00	31.06	D
	ATOM	6769	O	ALA	D	399	147.208	-5.469	35.041	1.00	29.92	D
	ATOM	6770	N	ASP	D	400	146.511	-7.083	36.444	1.00	33.65	D
	ATOM	6771	CA	ASP	D	400	147.767	-7.066	37.178	1.00	35.36	D
25	ATOM	6772	CB	ASP	D	400	147.670	-7.891	38.473	1.00	37.51	D
	ATOM	6773	CG	ASP	D	400	148.845	-7.626	39.429	1.00	42.78	D
	ATOM	6774	OD1	ASP	D	400	149.073	-6.446	39.813	1.00	42.00	D
	ATOM	6775	OD2	ASP	D	400	149.544	-8.603	39.802	1.00	45.77	D
	ATOM	6776	C	ASP	D	400	148.818	-7.639	36.237	1.00	34.42	D
30	ATOM	6777	O	ASP	D	400	149.996	-7.735	36.579	1.00	34.18	D
	ATOM	6778	N	ASP	D	401	148.379	-8.014	35.037	1.00	33.68	D
	ATOM	6779	CA	ASP	D	401	149.293	-8.550	34.047	1.00	32.54	D
	ATOM	6780	CB	ASP	D	401	148.571	-9.554	33.118	1.00	31.92	D
	ATOM	6781	CG	ASP	D	401	147.897	-8.910	31.909	1.00	31.59	D
35	ATOM	6782	OD1	ASP	D	401	147.579	-7.704	31.945	1.00	30.42	D
	ATOM	6783	OD2	ASP	D	401	147.671	-9.645	30.916	1.00	31.10	D
	ATOM	6784	C	ASP	D	401	149.901	-7.372	33.293	1.00	32.98	D
	ATOM	6785	O	ASP	D	401	150.551	-7.539	32.266	1.00	33.47	D
	ATOM	6786	N	LYS	D	402	149.699	-6.180	33.854	1.00	33.97	D
40	ATOM	6787	CA	LYS	D	402	150.215	-4.921	33.319	1.00	34.64	D
	ATOM	6788	CB	LYS	D	402	151.735	-4.825	33.568	1.00	33.75	D
	ATOM	6789	CG	LYS	D	402	152.545	-5.988	33.073	1.00	33.34	D
	ATOM	6790	CD	LYS	D	402	153.625	-6.377	34.058	1.00	34.65	D
	ATOM	6791	CE	LYS	D	402	154.661	-5.300	34.221	1.00	35.08	D
45	ATOM	6792	NZ	LYS	D	402	155.714	-5.811	35.142	1.00	34.72	D
	ATOM	6793	C	LYS	D	402	149.895	-4.650	31.846	1.00	35.07	D
	ATOM	6794	O	LYS	D	402	150.606	-3.907	31.167	1.00	35.57	D
	ATOM	6795	N	MSE	D	403	148.809	-5.238	31.360	1.00	37.46	D
	ATOM	6796	CA	MSE	D	403	148.389	-5.066	29.966	1.00	39.42	D
50	ATOM	6797	CB	MSE	D	403	148.429	-6.405	29.210	1.00	40.61	D
	ATOM	6798	CG	MSE	D	403	149.792	-7.054	29.119	1.00	42.82	D
	ATOM	6799	SE	MSE	D	403	150.956	-5.997	28.018	1.00	47.96	D
	ATOM	6800	CE	MSE	D	403	152.415	-5.649	29.261	1.00	46.83	D
	ATOM	6801	C	MSE	D	403	146.970	-4.518	29.882	1.00	39.22	D

	ATOM	6802	O	MSE	D	403	146.140	-4.767	30.761	1.00	41.64	D
	ATOM	6803	N	ILE	D	404	146.691	-3.797	28.802	1.00	37.92	D
	ATOM	6804	CA	ILE	D	404	145.372	-3.216	28.582	1.00	35.96	D
	ATOM	6805	CB	ILE	D	404	145.455	-1.675	28.574	1.00	34.69	D
5	ATOM	6806	CG2	ILE	D	404	144.114	-1.082	28.156	1.00	33.19	D
	ATOM	6807	CG1	ILE	D	404	145.880	-1.186	29.962	1.00	33.10	D
	ATOM	6808	CD1	ILE	D	404	146.272	0.266	29.999	1.00	31.33	D
	ATOM	6809	C	ILE	D	404	144.788	-3.709	27.251	1.00	35.14	D
	ATOM	6810	O	ILE	D	404	145.304	-3.392	26.193	1.00	34.48	D
10	ATOM	6811	N	ARG	D	405	143.709	-4.482	27.325	1.00	34.81	D
	ATOM	6812	CA	ARG	D	405	143.046	-5.027	26.151	1.00	34.51	D
	ATOM	6813	CB	ARG	D	405	142.428	-6.373	26.494	1.00	34.25	D
	ATOM	6814	CG	ARG	D	405	143.353	-7.285	27.227	1.00	34.29	D
	ATOM	6815	CD	ARG	D	405	144.147	-8.101	26.302	1.00	33.92	D
15	ATOM	6816	NE	ARG	D	405	143.362	-9.187	25.745	1.00	34.85	D
	ATOM	6817	CZ	ARG	D	405	143.844	-10.076	24.882	1.00	37.01	D
	ATOM	6818	NH1	ARG	D	405	145.110	-9.992	24.481	1.00	32.55	D
	ATOM	6819	NH2	ARG	D	405	143.069	-11.063	24.436	1.00	38.58	D
	ATOM	6820	C	ARG	D	405	141.931	-4.099	25.668	1.00	35.40	D
20	ATOM	6821	O	ARG	D	405	141.238	-3.474	26.479	1.00	36.54	D
	ATOM	6822	N	VAL	D	406	141.749	-4.041	24.349	1.00	35.29	D
	ATOM	6823	CA	VAL	D	406	140.719	-3.214	23.719	1.00	34.73	D
	ATOM	6824	CB	VAL	D	406	141.332	-2.093	22.879	1.00	35.48	D
	ATOM	6825	CG1	VAL	D	406	140.229	-1.244	22.275	1.00	35.19	D
25	ATOM	6826	CG2	VAL	D	406	142.275	-1.253	23.737	1.00	35.51	D
	ATOM	6827	C	VAL	D	406	139.921	-4.085	22.780	1.00	34.43	D
	ATOM	6828	O	VAL	D	406	140.500	-4.664	21.874	1.00	34.33	D
	ATOM	6829	N	TYR	D	407	138.603	-4.160	22.977	1.00	34.53	D
	ATOM	6830	CA	TYR	D	407	137.739	-4.985	22.124	1.00	34.18	D
30	ATOM	6831	CB	TYR	D	407	137.059	-6.091	22.937	1.00	33.29	D
	ATOM	6832	CG	TYR	D	407	137.966	-6.948	23.781	1.00	33.16	D
	ATOM	6833	CD1	TYR	D	407	138.423	-6.509	25.026	1.00	32.93	D
	ATOM	6834	CE1	TYR	D	407	139.255	-7.313	25.802	1.00	33.43	D
	ATOM	6835	CD2	TYR	D	407	138.362	-8.206	23.335	1.00	31.85	D
35	ATOM	6836	CE2	TYR	D	407	139.189	-9.013	24.091	1.00	31.74	D
	ATOM	6837	CZ	TYR	D	407	139.637	-8.572	25.320	1.00	33.54	D
	ATOM	6838	OH	TYR	D	407	140.485	-9.378	26.052	1.00	34.77	D
	ATOM	6839	C	TYR	D	407	136.635	-4.194	21.417	1.00	34.58	D
	ATOM	6840	O	TYR	D	407	136.246	-3.117	21.864	1.00	35.32	D
40	ATOM	6841	N	ASP	D	408	136.122	-4.775	20.332	1.00	35.38	D
	ATOM	6842	CA	ASP	D	408	135.043	-4.221	19.501	1.00	35.74	D
	ATOM	6843	CB	ASP	D	408	135.302	-4.625	18.038	1.00	38.38	D
	ATOM	6844	CG	ASP	D	408	134.214	-4.143	17.066	1.00	40.45	D
	ATOM	6845	OD1	ASP	D	408	133.015	-4.143	17.433	1.00	41.61	D
45	ATOM	6846	OD2	ASP	D	408	134.563	-3.781	15.917	1.00	39.05	D
	ATOM	6847	C	ASP	D	408	133.685	-4.788	19.965	1.00	35.67	D
	ATOM	6848	O	ASP	D	408	133.413	-5.980	19.799	1.00	35.45	D
	ATOM	6849	N	SER	D	409	132.829	-3.934	20.519	1.00	36.24	D
	ATOM	6850	CA	SER	D	409	131.510	-4.351	21.021	1.00	37.97	D
50	ATOM	6851	CB	SER	D	409	130.779	-3.160	21.623	1.00	39.00	D
	ATOM	6852	OG	SER	D	409	131.590	-2.452	22.533	1.00	42.40	D
	ATOM	6853	C	SER	D	409	130.594	-4.953	19.968	1.00	39.04	D
	ATOM	6854	O	SER	D	409	129.915	-5.958	20.216	1.00	38.64	D
	ATOM	6855	N	ILE	D	410	130.565	-4.295	18.807	1.00	40.27	D

	ATOM	6856	CA	ILE	D	410	129.740	-4.695	17.658	1.00	41.19	D
	ATOM	6857	CB	ILE	D	410	129.743	-3.613	16.553	1.00	42.29	D
	ATOM	6858	CG2	ILE	D	410	128.654	-3.904	15.539	1.00	41.48	D
	ATOM	6859	CG1	ILE	D	410	129.507	-2.227	17.162	1.00	43.94	D
5	ATOM	6860	CD1	ILE	D	410	129.838	-1.089	16.202	1.00	43.04	D
	ATOM	6861	C	ILE	D	410	130.244	-5.996	17.038	1.00	40.21	D
	ATOM	6862	O	ILE	D	410	129.616	-7.041	17.170	1.00	40.47	D
	ATOM	6863	N	ASN	D	411	131.385	-5.945	16.370	1.00	38.97	D
	ATOM	6864	CA	ASN	D	411	131.900	-7.153	15.769	1.00	39.16	D
10	ATOM	6865	CB	ASN	D	411	133.158	-6.848	14.985	1.00	41.69	D
	ATOM	6866	CG	ASN	D	411	132.943	-5.731	13.995	1.00	43.77	D
	ATOM	6867	OD1	ASN	D	411	131.889	-5.649	13.355	1.00	43.07	D
	ATOM	6868	ND2	ASN	D	411	133.938	-4.866	13.855	1.00	45.58	D
	ATOM	6869	C	ASN	D	411	132.178	-8.213	16.805	1.00	38.20	D
15	ATOM	6870	O	ASN	D	411	132.364	-9.377	16.458	1.00	36.34	D
	ATOM	6871	N	LYS	D	412	132.197	-7.800	18.074	1.00	37.74	D
	ATOM	6872	CA	LYS	D	412	132.451	-8.693	19.211	1.00	36.63	D
	ATOM	6873	CB	LYS	D	412	131.300	-9.690	19.338	1.00	35.83	D
	ATOM	6874	CG	LYS	D	412	129.936	-9.018	19.314	1.00	35.16	D
20	ATOM	6875	CD	LYS	D	412	128.805	-10.011	19.175	1.00	34.88	D
	ATOM	6876	CE	LYS	D	412	127.483	-9.278	19.119	1.00	36.26	D
	ATOM	6877	NZ	LYS	D	412	126.321	-10.211	19.101	1.00	37.05	D
	ATOM	6878	C	LYS	D	412	133.776	-9.442	19.066	1.00	36.14	D
	ATOM	6879	O	LYS	D	412	133.828	-10.659	19.227	1.00	35.34	D
25	ATOM	6880	N	LYS	D	413	134.845	-8.707	18.772	1.00	36.48	D
	ATOM	6881	CA	LYS	D	413	136.161	-9.314	18.597	1.00	38.12	D
	ATOM	6882	CB	LYS	D	413	136.440	-9.573	17.118	1.00	37.83	D
	ATOM	6883	CG	LYS	D	413	136.378	-8.322	16.257	1.00	41.43	D
	ATOM	6884	CD	LYS	D	413	136.964	-8.566	14.853	1.00	44.72	D
30	ATOM	6885	CE	LYS	D	413	136.674	-7.400	13.885	1.00	46.65	D
	ATOM	6886	NZ	LYS	D	413	137.132	-6.056	14.371	1.00	47.55	D
	ATOM	6887	C	LYS	D	413	137.303	-8.471	19.159	1.00	38.78	D
	ATOM	6888	O	LYS	D	413	137.244	-7.242	19.151	1.00	38.60	D
	ATOM	6889	N	PHE	D	414	138.348	-9.149	19.630	1.00	38.98	D
35	ATOM	6890	CA	PHE	D	414	139.520	-8.489	20.191	1.00	38.98	D
	ATOM	6891	CB	PHE	D	414	140.513	-9.528	20.715	1.00	39.56	D
	ATOM	6892	CG	PHE	D	414	141.908	-8.997	20.902	1.00	41.07	D
	ATOM	6893	CD1	PHE	D	414	142.184	-8.046	21.874	1.00	43.51	D
	ATOM	6894	CD2	PHE	D	414	142.949	-9.454	20.110	1.00	41.71	D
40	ATOM	6895	CE1	PHE	D	414	143.488	-7.557	22.058	1.00	44.32	D
	ATOM	6896	CE2	PHE	D	414	144.251	-8.973	20.287	1.00	43.60	D
	ATOM	6897	CZ	PHE	D	414	144.519	-8.022	21.264	1.00	42.78	D
	ATOM	6898	C	PHE	D	414	140.208	-7.620	19.157	1.00	39.17	D
	ATOM	6899	O	PHE	D	414	140.529	-8.083	18.068	1.00	40.84	D
45	ATOM	6900	N	LEU	D	415	140.430	-6.359	19.506	1.00	38.34	D
	ATOM	6901	CA	LEU	D	415	141.099	-5.434	18.617	1.00	37.48	D
	ATOM	6902	CB	LEU	D	415	140.555	-4.026	18.815	1.00	37.15	D
	ATOM	6903	CG	LEU	D	415	139.163	-3.792	18.224	1.00	38.52	D
	ATOM	6904	CD1	LEU	D	415	138.737	-2.351	18.453	1.00	39.38	D
50	ATOM	6905	CD2	LEU	D	415	139.191	-4.091	16.736	1.00	39.17	D
	ATOM	6906	C	LEU	D	415	142.611	-5.451	18.832	1.00	37.67	D
	ATOM	6907	O	LEU	D	415	143.328	-6.171	18.138	1.00	38.98	D
	ATOM	6908	N	LEU	D	416	143.097	-4.681	19.799	1.00	35.95	D
	ATOM	6909	CA	LEU	D	416	144.528	-4.611	20.052	1.00	34.61	D

	ATOM	6910	CB	LEU	D	416	145.102	-3.394	19.317	1.00	32.51	D
	ATOM	6911	CG	LEU	D	416	144.656	-2.045	19.880	1.00	30.50	D
	ATOM	6912	CD1	LEU	D	416	145.700	-1.579	20.853	1.00	31.53	D
	ATOM	6913	CD2	LEU	D	416	144.470	-1.017	18.789	1.00	30.55	D
5	ATOM	6914	C	LEU	D	416	144.865	-4.519	21.545	1.00	35.53	D
	ATOM	6915	O	LEU	D	416	144.013	-4.200	22.364	1.00	36.55	D
	ATOM	6916	N	GLN	D	417	146.116	-4.791	21.891	1.00	35.81	D
	ATOM	6917	CA	GLN	D	417	146.547	-4.716	23.271	1.00	35.57	D
	ATOM	6918	CB	GLN	D	417	147.254	-6.007	23.671	1.00	37.43	D
10	ATOM	6919	CG	GLN	D	417	147.625	-6.074	25.145	1.00	39.62	D
	ATOM	6920	CD	GLN	D	417	148.512	-7.253	25.464	1.00	41.04	D
	ATOM	6921	OE1	GLN	D	417	149.615	-7.378	24.914	1.00	43.24	D
	ATOM	6922	NE2	GLN	D	417	148.046	-8.128	26.358	1.00	40.41	D
	ATOM	6923	C	GLN	D	417	147.506	-3.532	23.450	1.00	35.61	D
15	ATOM	6924	O	GLN	D	417	148.374	-3.297	22.605	1.00	35.43	D
	ATOM	6925	N	LEU	D	418	147.337	-2.798	24.551	1.00	35.15	D
	ATOM	6926	CA	LEU	D	418	148.166	-1.644	24.885	1.00	33.41	D
	ATOM	6927	CB	LEU	D	418	147.315	-0.523	25.429	1.00	31.33	D
	ATOM	6928	CG	LEU	D	418	146.413	0.034	24.359	1.00	31.84	D
20	ATOM	6929	CD1	LEU	D	418	145.508	1.119	24.943	1.00	33.02	D
	ATOM	6930	CD2	LEU	D	418	147.293	0.595	23.253	1.00	33.13	D
	ATOM	6931	C	LEU	D	418	149.180	-2.006	25.939	1.00	33.92	D
	ATOM	6932	O	LEU	D	418	148.811	-2.281	27.076	1.00	33.63	D
	ATOM	6933	N	SER	D	419	150.458	-1.991	25.572	1.00	35.50	D
25	ATOM	6934	CA	SER	D	419	151.529	-2.323	26.518	1.00	35.75	D
	ATOM	6935	CB	SER	D	419	152.504	-3.304	25.889	1.00	36.24	D
	ATOM	6936	OG	SER	D	419	153.366	-2.611	25.006	1.00	39.10	D
	ATOM	6937	C	SER	D	419	152.286	-1.060	26.903	1.00	34.65	D
	ATOM	6938	O	SER	D	419	152.148	-0.036	26.243	1.00	35.71	D
30	ATOM	6939	N	GLY	D	420	153.082	-1.132	27.969	1.00	34.21	D
	ATOM	6940	CA	GLY	D	420	153.845	0.030	28.407	1.00	32.81	D
	ATOM	6941	C	GLY	D	420	154.127	0.063	29.904	1.00	32.19	D
	ATOM	6942	O	GLY	D	420	155.277	0.111	30.334	1.00	32.95	D
	ATOM	6943	N	HIS	D	421	153.057	0.038	30.690	1.00	32.53	D
35	ATOM	6944	CA	HIS	D	421	153.116	0.056	32.142	1.00	31.89	D
	ATOM	6945	CB	HIS	D	421	151.744	-0.233	32.728	1.00	28.17	D
	ATOM	6946	CG	HIS	D	421	150.862	0.972	32.856	1.00	26.59	D
	ATOM	6947	CD2	HIS	D	421	149.677	1.270	32.274	1.00	23.86	D
	ATOM	6948	ND1	HIS	D	421	151.123	1.998	33.738	1.00	24.07	D
40	ATOM	6949	CE1	HIS	D	421	150.133	2.872	33.699	1.00	24.39	D
	ATOM	6950	NE2	HIS	D	421	149.243	2.454	32.818	1.00	22.81	D
	ATOM	6951	C	HIS	D	421	154.082	-0.966	32.714	1.00	34.84	D
	ATOM	6952	O	HIS	D	421	154.005	-2.162	32.399	1.00	35.95	D
	ATOM	6953	N	ASP	D	422	154.973	-0.487	33.580	1.00	37.06	D
45	ATOM	6954	CA	ASP	D	422	155.969	-1.328	34.241	1.00	37.22	D
	ATOM	6955	CB	ASP	D	422	157.181	-0.481	34.655	1.00	37.19	D
	ATOM	6956	CG	ASP	D	422	157.811	0.261	33.479	1.00	38.07	D
	ATOM	6957	OD1	ASP	D	422	158.398	-0.414	32.605	1.00	36.97	D
	ATOM	6958	OD2	ASP	D	422	157.716	1.519	33.426	1.00	39.00	D
50	ATOM	6959	C	ASP	D	422	155.331	-1.974	35.468	1.00	37.57	D
	ATOM	6960	O	ASP	D	422	155.947	-2.791	36.155	1.00	38.18	D
	ATOM	6961	N	GLY	D	423	154.089	-1.584	35.735	1.00	38.03	D
	ATOM	6962	CA	GLY	D	423	153.357	-2.135	36.862	1.00	37.36	D
	ATOM	6963	C	GLY	D	423	151.963	-2.599	36.451	1.00	36.40	D

	ATOM	6964	O	GLY	D	423	151.496	-2.282	35.358	1.00	37.00	D
	ATOM	6965	N	GLY	D	424	151.297	-3.361	37.311	1.00	35.05	D
	ATOM	6966	CA	GLY	D	424	149.965	-3.823	36.984	1.00	33.45	D
	ATOM	6967	C	GLY	D	424	149.032	-2.637	36.920	1.00	33.03	D
5	ATOM	6968	O	GLY	D	424	149.183	-1.692	37.687	1.00	32.43	D
	ATOM	6969	N	VAL	D	425	148.074	-2.685	36.004	1.00	33.29	D
	ATOM	6970	CA	VAL	D	425	147.112	-1.602	35.826	1.00	34.26	D
	ATOM	6971	CB	VAL	D	425	146.545	-1.623	34.420	1.00	34.93	D
	ATOM	6972	CG1	VAL	D	425	145.785	-0.328	34.150	1.00	37.13	D
10	ATOM	6973	CG2	VAL	D	425	147.661	-1.843	33.433	1.00	34.83	D
	ATOM	6974	C	VAL	D	425	145.955	-1.776	36.795	1.00	33.41	D
	ATOM	6975	O	VAL	D	425	145.473	-2.880	36.975	1.00	33.61	D
	ATOM	6976	N	TRP	D	426	145.493	-0.700	37.410	1.00	32.49	D
	ATOM	6977	CA	TRP	D	426	144.395	-0.837	38.343	1.00	32.03	D
15	ATOM	6978	CB	TRP	D	426	144.952	-0.866	39.774	1.00	30.72	D
	ATOM	6979	CG	TRP	D	426	145.618	-2.192	40.132	1.00	29.46	D
	ATOM	6980	CD2	TRP	D	426	145.011	-3.288	40.834	1.00	27.59	D
	ATOM	6981	CE2	TRP	D	426	145.982	-4.311	40.937	1.00	25.67	D
	ATOM	6982	CE3	TRP	D	426	143.738	-3.502	41.390	1.00	27.62	D
20	ATOM	6983	CD1	TRP	D	426	146.903	-2.592	39.838	1.00	28.36	D
	ATOM	6984	NE1	TRP	D	426	147.122	-3.863	40.321	1.00	26.42	D
	ATOM	6985	CZ2	TRP	D	426	145.720	-5.527	41.572	1.00	23.76	D
	ATOM	6986	CZ3	TRP	D	426	143.477	-4.712	42.021	1.00	25.66	D
	ATOM	6987	CH2	TRP	D	426	144.467	-5.711	42.108	1.00	24.10	D
25	ATOM	6988	C	TRP	D	426	143.291	0.224	38.190	1.00	32.39	D
	ATOM	6989	O	TRP	D	426	142.270	0.182	38.876	1.00	32.60	D
	ATOM	6990	N	ALA	D	427	143.483	1.164	37.275	1.00	31.70	D
	ATOM	6991	CA	ALA	D	427	142.489	2.201	37.060	1.00	32.14	D
	ATOM	6992	CB	ALA	D	427	142.699	3.330	38.059	1.00	30.77	D
30	ATOM	6993	C	ALA	D	427	142.544	2.749	35.631	1.00	32.54	D
	ATOM	6994	O	ALA	D	427	143.610	3.128	35.148	1.00	33.11	D
	ATOM	6995	N	LEU	D	428	141.403	2.763	34.949	1.00	31.96	D
	ATOM	6996	CA	LEU	D	428	141.362	3.298	33.605	1.00	31.52	D
	ATOM	6997	CB	LEU	D	428	141.879	2.273	32.591	1.00	30.47	D
35	ATOM	6998	CG	LEU	D	428	141.523	0.793	32.619	1.00	25.70	D
	ATOM	6999	CD1	LEU	D	428	140.061	0.566	32.426	1.00	26.95	D
	ATOM	7000	CD2	LEU	D	428	142.302	0.127	31.520	1.00	26.15	D
	ATOM	7001	C	LEU	D	428	139.998	3.823	33.185	1.00	32.41	D
	ATOM	7002	O	LEU	D	428	139.015	3.092	33.159	1.00	31.99	D
40	ATOM	7003	N	LYS	D	429	139.970	5.117	32.874	1.00	34.44	D
	ATOM	7004	CA	LYS	D	429	138.779	5.846	32.441	1.00	36.04	D
	ATOM	7005	CB	LYS	D	429	138.655	7.149	33.247	1.00	36.79	D
	ATOM	7006	CG	LYS	D	429	137.379	7.954	33.000	1.00	41.16	D
	ATOM	7007	CD	LYS	D	429	136.228	7.499	33.914	1.00	44.67	D
45	ATOM	7008	CE	LYS	D	429	134.828	7.936	33.399	1.00	47.43	D
	ATOM	7009	NZ	LYS	D	429	134.385	7.223	32.133	1.00	49.62	D
	ATOM	7010	C	LYS	D	429	138.944	6.184	30.951	1.00	35.80	D
	ATOM	7011	O	LYS	D	429	139.982	6.698	30.531	1.00	35.22	D
	ATOM	7012	N	TYR	D	430	137.926	5.888	30.152	1.00	36.71	D
50	ATOM	7013	CA	TYR	D	430	137.962	6.183	28.719	1.00	38.50	D
	ATOM	7014	CB	TYR	D	430	137.142	5.152	27.936	1.00	38.31	D
	ATOM	7015	CG	TYR	D	430	136.840	5.560	26.501	1.00	38.68	D
	ATOM	7016	CD1	TYR	D	430	135.713	6.331	26.192	1.00	38.18	D
	ATOM	7017	CE1	TYR	D	430	135.427	6.702	24.875	1.00	37.22	D

	ATOM	7018	CD2	TYR	D	430	137.680	5.173	25.449	1.00	39.59	D
	ATOM	7019	CE2	TYR	D	430	137.403	5.542	24.126	1.00	38.38	D
	ATOM	7020	CZ	TYR	D	430	136.275	6.303	23.853	1.00	38.21	D
	ATOM	7021	OH	TYR	D	430	135.983	6.646	22.557	1.00	37.82	D
5	ATOM	7022	C	TYR	D	430	137.401	7.574	28.427	1.00	39.86	D
	ATOM	7023	O	TYR	D	430	136.344	7.931	28.934	1.00	39.99	D
	ATOM	7024	N	ALA	D	431	138.109	8.349	27.607	1.00	40.69	D
	ATOM	7025	CA	ALA	D	431	137.660	9.688	27.227	1.00	41.42	D
	ATOM	7026	CB	ALA	D	431	138.790	10.695	27.407	1.00	40.10	D
10	ATOM	7027	C	ALA	D	431	137.208	9.641	25.763	1.00	43.09	D
	ATOM	7028	O	ALA	D	431	137.842	8.998	24.916	1.00	43.69	D
	ATOM	7029	N	HIS	D	432	136.108	10.321	25.465	1.00	42.71	D
	ATOM	7030	CA	HIS	D	432	135.584	10.340	24.102	1.00	43.16	D
	ATOM	7031	CB	HIS	D	432	134.468	11.383	23.966	1.00	47.95	D
15	ATOM	7032	CG	HIS	D	432	133.942	11.523	22.566	1.00	53.08	D
	ATOM	7033	CD2	HIS	D	432	133.728	12.622	21.801	1.00	53.58	D
	ATOM	7034	ND1	HIS	D	432	133.594	10.439	21.787	1.00	53.70	D
	ATOM	7035	CE1	HIS	D	432	133.192	10.865	20.601	1.00	54.74	D
	ATOM	7036	NE2	HIS	D	432	133.265	12.184	20.584	1.00	54.71	D
20	ATOM	7037	C	HIS	D	432	136.646	10.636	23.052	1.00	40.32	D
	ATOM	7038	O	HIS	D	432	137.420	11.573	23.201	1.00	40.89	D
	ATOM	7039	N	GLY	D	433	136.669	9.852	21.980	1.00	37.59	D
	ATOM	7040	CA	GLY	D	433	137.640	10.095	20.926	1.00	36.16	D
	ATOM	7041	C	GLY	D	433	138.701	9.029	20.850	1.00	34.81	D
25	ATOM	7042	O	GLY	D	433	139.697	9.177	20.143	1.00	32.92	D
	ATOM	7043	N	GLY	D	434	138.474	7.948	21.588	1.00	36.25	D
	ATOM	7044	CA	GLY	D	434	139.412	6.841	21.617	1.00	36.22	D
	ATOM	7045	C	GLY	D	434	140.580	7.079	22.557	1.00	36.76	D
	ATOM	7046	O	GLY	D	434	141.559	6.338	22.493	1.00	37.12	D
30	ATOM	7047	N	ILE	D	435	140.469	8.106	23.411	1.00	37.42	D
	ATOM	7048	CA	ILE	D	435	141.501	8.478	24.397	1.00	37.95	D
	ATOM	7049	CB	ILE	D	435	141.424	9.992	24.784	1.00	39.16	D
	ATOM	7050	CG2	ILE	D	435	142.684	10.430	25.539	1.00	37.49	D
	ATOM	7051	CG1	ILE	D	435	141.328	10.839	23.519	1.00	39.15	D
35	ATOM	7052	CD1	ILE	D	435	142.476	10.580	22.572	1.00	38.06	D
	ATOM	7053	C	ILE	D	435	141.273	7.662	25.658	1.00	37.16	D
	ATOM	7054	O	ILE	D	435	140.130	7.426	26.059	1.00	36.94	D
	ATOM	7055	N	LEU	D	436	142.360	7.251	26.297	1.00	35.58	D
	ATOM	7056	CA	LEU	D	436	142.243	6.427	27.481	1.00	34.59	D
40	ATOM	7057	CB	LEU	D	436	142.354	4.980	27.046	1.00	35.11	D
	ATOM	7058	CG	LEU	D	436	141.894	3.866	27.965	1.00	35.32	D
	ATOM	7059	CD1	LEU	D	436	142.000	2.560	27.178	1.00	34.07	D
	ATOM	7060	CD2	LEU	D	436	142.727	3.819	29.234	1.00	35.01	D
	ATOM	7061	C	LEU	D	436	143.309	6.742	28.511	1.00	34.64	D
45	ATOM	7062	O	LEU	D	436	144.495	6.786	28.195	1.00	35.84	D
	ATOM	7063	N	VAL	D	437	142.891	6.960	29.750	1.00	33.63	D
	ATOM	7064	CA	VAL	D	437	143.854	7.244	30.801	1.00	32.09	D
	ATOM	7065	CB	VAL	D	437	143.484	8.519	31.575	1.00	31.66	D
	ATOM	7066	CG1	VAL	D	437	144.624	8.902	32.506	1.00	32.49	D
50	ATOM	7067	CG2	VAL	D	437	143.172	9.650	30.608	1.00	31.31	D
	ATOM	7068	C	VAL	D	437	143.887	6.058	31.764	1.00	31.94	D
	ATOM	7069	O	VAL	D	437	142.845	5.454	32.047	1.00	31.55	D
	ATOM	7070	N	SER	D	438	145.080	5.707	32.246	1.00	29.85	D
	ATOM	7071	CA	SER	D	438	145.201	4.597	33.189	1.00	26.33	D

	ATOM	7072	CB	SER	D	438	145.601	3.302	32.480	1.00	25.65	D
	ATOM	7073	OG	SER	D	438	146.858	3.426	31.852	1.00	26.66	D
	ATOM	7074	C	SER	D	438	146.156	4.853	34.336	1.00	23.90	D
	ATOM	7075	O	SER	D	438	146.977	5.765	34.294	1.00	21.89	D
5	ATOM	7076	N	GLY	D	439	146.019	4.025	35.366	1.00	23.29	D
	ATOM	7077	CA	GLY	D	439	146.835	4.130	36.563	1.00	23.55	D
	ATOM	7078	C	GLY	D	439	147.396	2.783	36.962	1.00	23.12	D
	ATOM	7079	O	GLY	D	439	146.725	1.748	36.883	1.00	22.22	D
	ATOM	7080	N	SER	D	440	148.634	2.800	37.429	1.00	23.85	D
10	ATOM	7081	CA	SER	D	440	149.302	1.562	37.786	1.00	25.71	D
	ATOM	7082	CB	SER	D	440	150.244	1.169	36.630	1.00	24.70	D
	ATOM	7083	OG	SER	D	440	151.145	0.129	36.979	1.00	23.47	D
	ATOM	7084	C	SER	D	440	150.078	1.620	39.099	1.00	26.18	D
	ATOM	7085	O	SER	D	440	150.112	2.651	39.793	1.00	26.21	D
15	ATOM	7086	N	THR	D	441	150.695	0.481	39.413	1.00	27.38	D
	ATOM	7087	CA	THR	D	441	151.521	0.308	40.593	1.00	27.39	D
	ATOM	7088	CB	THR	D	441	151.676	-1.165	40.968	1.00	28.12	D
	ATOM	7089	OG1	THR	D	441	152.519	-1.810	40.004	1.00	27.63	D
	ATOM	7090	CG2	THR	D	441	150.310	-1.858	41.003	1.00	28.73	D
20	ATOM	7091	C	THR	D	441	152.903	0.847	40.237	1.00	28.31	D
	ATOM	7092	O	THR	D	441	153.768	0.906	41.090	1.00	29.00	D
	ATOM	7093	N	ASP	D	442	153.116	1.234	38.980	1.00	29.46	D
	ATOM	7094	CA	ASP	D	442	154.402	1.796	38.603	1.00	31.38	D
	ATOM	7095	CB	ASP	D	442	154.724	1.551	37.126	1.00	33.65	D
25	ATOM	7096	CG	ASP	D	442	153.695	2.167	36.185	1.00	35.87	D
	ATOM	7097	OD1	ASP	D	442	152.845	2.962	36.680	1.00	35.07	D
	ATOM	7098	OD2	ASP	D	442	153.753	1.860	34.959	1.00	34.85	D
	ATOM	7099	C	ASP	D	442	154.351	3.287	38.857	1.00	31.58	D
	ATOM	7100	O	ASP	D	442	155.161	4.049	38.334	1.00	31.31	D
30	ATOM	7101	N	ARG	D	443	153.360	3.700	39.635	1.00	31.79	D
	ATOM	7102	CA	ARG	D	443	153.191	5.100	39.983	1.00	31.82	D
	ATOM	7103	CB	ARG	D	443	154.413	5.569	40.760	1.00	28.96	D
	ATOM	7104	CG	ARG	D	443	154.805	4.604	41.846	1.00	26.68	D
	ATOM	7105	CD	ARG	D	443	156.056	5.065	42.541	1.00	25.25	D
35	ATOM	7106	NE	ARG	D	443	156.496	4.111	43.541	1.00	26.33	D
	ATOM	7107	CZ	ARG	D	443	157.552	4.303	44.319	1.00	27.22	D
	ATOM	7108	NH1	ARG	D	443	158.250	5.419	44.192	1.00	28.58	D
	ATOM	7109	NH2	ARG	D	443	157.916	3.388	45.213	1.00	26.32	D
	ATOM	7110	C	ARG	D	443	152.955	6.016	38.783	1.00	32.05	D
40	ATOM	7111	O	ARG	D	443	152.975	7.243	38.917	1.00	32.48	D
	ATOM	7112	N	THR	D	444	152.705	5.439	37.616	1.00	31.82	D
	ATOM	7113	CA	THR	D	444	152.486	6.283	36.459	1.00	32.99	D
	ATOM	7114	CB	THR	D	444	153.335	5.824	35.246	1.00	32.98	D
	ATOM	7115	OG1	THR	D	444	152.768	4.643	34.657	1.00	30.88	D
45	ATOM	7116	CG2	THR	D	444	154.757	5.549	35.680	1.00	31.91	D
	ATOM	7117	C	THR	D	444	151.036	6.451	36.000	1.00	34.38	D
	ATOM	7118	O	THR	D	444	150.182	5.570	36.164	1.00	34.02	D
	ATOM	7119	N	VAL	D	445	150.784	7.623	35.432	1.00	35.02	D
	ATOM	7120	CA	VAL	D	445	149.492	7.992	34.888	1.00	35.88	D
50	ATOM	7121	CB	VAL	D	445	149.049	9.384	35.406	1.00	34.38	D
	ATOM	7122	CG1	VAL	D	445	147.839	9.871	34.640	1.00	33.91	D
	ATOM	7123	CG2	VAL	D	445	148.747	9.312	36.893	1.00	33.31	D
	ATOM	7124	C	VAL	D	445	149.787	8.067	33.392	1.00	38.00	D
	ATOM	7125	O	VAL	D	445	150.648	8.841	32.969	1.00	40.09	D

	ATOM	7126	N	ARG	D	446	149.116	7.256	32.583	1.00	38.70	D
	ATOM	7127	CA	ARG	D	446	149.390	7.299	31.152	1.00	40.25	D
	ATOM	7128	CB	ARG	D	446	150.102	6.016	30.707	1.00	40.97	D
	ATOM	7129	CG	ARG	D	446	151.387	5.796	31.448	1.00	42.38	D
5	ATOM	7130	CD	ARG	D	446	152.190	4.636	30.925	1.00	44.42	D
	ATOM	7131	NE	ARG	D	446	153.302	4.360	31.835	1.00	48.85	D
	ATOM	7132	CZ	ARG	D	446	154.291	3.506	31.588	1.00	50.95	D
	ATOM	7133	NH1	ARG	D	446	154.316	2.834	30.442	1.00	52.13	D
	ATOM	7134	NH2	ARG	D	446	155.251	3.320	32.490	1.00	51.46	D
10	ATOM	7135	C	ARG	D	446	148.155	7.527	30.296	1.00	40.71	D
	ATOM	7136	O	ARG	D	446	147.050	7.083	30.635	1.00	39.57	D
	ATOM	7137	N	VAL	D	447	148.357	8.253	29.195	1.00	40.90	D
	ATOM	7138	CA	VAL	D	447	147.293	8.552	28.237	1.00	41.54	D
	ATOM	7139	CB	VAL	D	447	147.260	10.037	27.849	1.00	40.47	D
15	ATOM	7140	CG1	VAL	D	447	146.043	10.306	26.981	1.00	38.69	D
	ATOM	7141	CG2	VAL	D	447	147.226	10.895	29.100	1.00	40.93	D
	ATOM	7142	C	VAL	D	447	147.566	7.735	26.991	1.00	42.31	D
	ATOM	7143	O	VAL	D	447	148.689	7.712	26.501	1.00	43.98	D
	ATOM	7144	N	TRP	D	448	146.549	7.055	26.481	1.00	42.01	D
20	ATOM	7145	CA	TRP	D	448	146.730	6.234	25.296	1.00	42.06	D
	ATOM	7146	CB	TRP	D	448	146.416	4.769	25.625	1.00	40.93	D
	ATOM	7147	CG	TRP	D	448	147.108	4.254	26.849	1.00	40.06	D
	ATOM	7148	CD2	TRP	D	448	148.167	3.294	26.890	1.00	39.39	D
	ATOM	7149	CE2	TRP	D	448	148.529	3.127	28.247	1.00	39.74	D
25	ATOM	7150	CE3	TRP	D	448	148.846	2.555	25.911	1.00	37.93	D
	ATOM	7151	CD1	TRP	D	448	146.871	4.621	28.145	1.00	39.85	D
	ATOM	7152	NE1	TRP	D	448	147.720	3.949	28.992	1.00	39.87	D
	ATOM	7153	CZ2	TRP	D	448	149.552	2.247	28.653	1.00	38.84	D
	ATOM	7154	CZ3	TRP	D	448	149.860	1.680	26.314	1.00	38.08	D
30	ATOM	7155	CH2	TRP	D	448	150.203	1.537	27.679	1.00	37.48	D
	ATOM	7156	C	TRP	D	448	145.825	6.705	24.156	1.00	42.74	D
	ATOM	7157	O	TRP	D	448	144.933	7.537	24.349	1.00	42.62	D
	ATOM	7158	N	ASP	D	449	146.067	6.165	22.967	1.00	43.66	D
	ATOM	7159	CA	ASP	D	449	145.265	6.485	21.797	1.00	44.36	D
35	ATOM	7160	CB	ASP	D	449	146.062	7.368	20.836	1.00	45.33	D
	ATOM	7161	CG	ASP	D	449	145.256	7.782	19.616	1.00	46.25	D
	ATOM	7162	OD1	ASP	D	449	145.791	8.522	18.771	1.00	46.26	D
	ATOM	7163	OD2	ASP	D	449	144.088	7.370	19.494	1.00	47.22	D
	ATOM	7164	C	ASP	D	449	144.899	5.169	21.119	1.00	44.82	D
40	ATOM	7165	O	ASP	D	449	145.735	4.551	20.468	1.00	44.81	D
	ATOM	7166	N	ILE	D	450	143.653	4.740	21.280	1.00	45.73	D
	ATOM	7167	CA	ILE	D	450	143.205	3.484	20.687	1.00	47.64	D
	ATOM	7168	CB	ILE	D	450	141.711	3.215	21.000	1.00	46.91	D
	ATOM	7169	CG2	ILE	D	450	141.335	1.820	20.527	1.00	45.80	D
45	ATOM	7170	CG1	ILE	D	450	141.455	3.357	22.507	1.00	46.32	D
	ATOM	7171	CD1	ILE	D	450	140.009	3.138	22.920	1.00	46.07	D
	ATOM	7172	C	ILE	D	450	143.395	3.516	19.173	1.00	49.71	D
	ATOM	7173	O	ILE	D	450	143.890	2.556	18.573	1.00	49.74	D
	ATOM	7174	N	LYS	D	451	142.984	4.631	18.571	1.00	51.95	D
50	ATOM	7175	CA	LYS	D	451	143.092	4.859	17.130	1.00	52.66	D
	ATOM	7176	CB	LYS	D	451	142.789	6.329	16.815	1.00	54.03	D
	ATOM	7177	CG	LYS	D	451	141.425	6.825	17.283	1.00	54.77	D
	ATOM	7178	CD	LYS	D	451	140.315	6.348	16.362	1.00	56.08	D
	ATOM	7179	CE	LYS	D	451	138.958	6.853	16.829	1.00	58.40	D

	ATOM	7180	NZ	LYS	D	451	138.564	6.293	18.170	1.00	60.81	D
	ATOM	7181	C	LYS	D	451	144.519	4.534	16.687	1.00	53.12	D
	ATOM	7182	O	LYS	D	451	144.743	3.637	15.875	1.00	52.92	D
	ATOM	7183	N	LYS	D	452	145.478	5.279	17.236	1.00	53.06	D
5	ATOM	7184	CA	LYS	D	452	146.889	5.081	16.922	1.00	53.16	D
	ATOM	7185	CB	LYS	D	452	147.727	6.274	17.405	1.00	54.65	D
	ATOM	7186	CG	LYS	D	452	147.432	7.608	16.705	1.00	55.78	D
	ATOM	7187	CD	LYS	D	452	148.434	8.689	17.106	1.00	54.91	D
	ATOM	7188	CE	LYS	D	452	148.269	9.952	16.262	1.00	56.24	D
10	ATOM	7189	NZ	LYS	D	452	146.931	10.592	16.394	1.00	55.58	D
	ATOM	7190	C	LYS	D	452	147.426	3.801	17.565	1.00	52.16	D
	ATOM	7191	O	LYS	D	452	148.530	3.352	17.257	1.00	52.14	D
	ATOM	7192	N	GLY	D	453	146.646	3.221	18.466	1.00	51.03	D
	ATOM	7193	CA	GLY	D	453	147.070	2.000	19.119	1.00	48.98	D
15	ATOM	7194	C	GLY	D	453	148.425	2.076	19.795	1.00	47.55	D
	ATOM	7195	O	GLY	D	453	149.268	1.206	19.598	1.00	48.41	D
	ATOM	7196	N	CYS	D	454	148.643	3.111	20.595	1.00	45.89	D
	ATOM	7197	CA	CYS	D	454	149.903	3.252	21.306	1.00	45.10	D
	ATOM	7198	CB	CYS	D	454	151.007	3.764	20.371	1.00	45.35	D
20	ATOM	7199	SG	CYS	D	454	151.016	5.592	20.180	1.00	46.05	D
	ATOM	7200	C	CYS	D	454	149.733	4.246	22.445	1.00	45.09	D
	ATOM	7201	O	CYS	D	454	148.660	4.827	22.632	1.00	43.95	D
	ATOM	7202	N	CYS	D	455	150.815	4.443	23.191	1.00	45.72	D
	ATOM	7203	CA	CYS	D	455	150.831	5.373	24.307	1.00	46.22	D
25	ATOM	7204	CB	CYS	D	455	151.663	4.818	25.461	1.00	46.14	D
	ATOM	7205	SG	CYS	D	455	151.652	5.917	26.902	1.00	44.91	D
	ATOM	7206	C	CYS	D	455	151.412	6.717	23.880	1.00	45.90	D
	ATOM	7207	O	CYS	D	455	152.504	6.787	23.328	1.00	45.72	D
	ATOM	7208	N	THR	D	456	150.674	7.778	24.160	1.00	46.41	D
30	ATOM	7209	CA	THR	D	456	151.089	9.114	23.807	1.00	47.30	D
	ATOM	7210	CB	THR	D	456	149.878	9.947	23.316	1.00	47.67	D
	ATOM	7211	OG1	THR	D	456	150.170	11.344	23.454	1.00	49.91	D
	ATOM	7212	CG2	THR	D	456	148.633	9.623	24.124	1.00	48.32	D
	ATOM	7213	C	THR	D	456	151.767	9.870	24.953	1.00	47.34	D
35	ATOM	7214	O	THR	D	456	152.722	10.614	24.729	1.00	47.57	D
	ATOM	7215	N	HIS	D	457	151.280	9.691	26.177	1.00	46.90	D
	ATOM	7216	CA	HIS	D	457	151.850	10.407	27.315	1.00	46.66	D
	ATOM	7217	CB	HIS	D	457	150.935	11.569	27.708	1.00	48.78	D
	ATOM	7218	CG	HIS	D	457	150.781	12.608	26.639	1.00	52.07	D
40	ATOM	7219	CD2	HIS	D	457	149.752	12.884	25.802	1.00	53.00	D
	ATOM	7220	ND1	HIS	D	457	151.768	13.525	26.349	1.00	51.90	D
	ATOM	7221	CE1	HIS	D	457	151.351	14.324	25.383	1.00	53.55	D
	ATOM	7222	NE2	HIS	D	457	150.131	13.957	25.033	1.00	53.69	D
	ATOM	7223	C	HIS	D	457	152.101	9.534	28.529	1.00	45.09	D
45	ATOM	7224	O	HIS	D	457	151.360	8.591	28.797	1.00	46.21	D
	ATOM	7225	N	VAL	D	458	153.163	9.864	29.255	1.00	43.08	D
	ATOM	7226	CA	VAL	D	458	153.544	9.142	30.462	1.00	40.12	D
	ATOM	7227	CB	VAL	D	458	154.847	8.350	30.247	1.00	38.48	D
	ATOM	7228	CG1	VAL	D	458	155.106	7.437	31.430	1.00	36.35	D
50	ATOM	7229	CG2	VAL	D	458	154.758	7.554	28.954	1.00	37.80	D
	ATOM	7230	C	VAL	D	458	153.761	10.197	31.535	1.00	38.68	D
	ATOM	7231	O	VAL	D	458	154.733	10.942	31.474	1.00	38.06	D
	ATOM	7232	N	PHE	D	459	152.834	10.267	32.491	1.00	37.03	D
	ATOM	7233	CA	PHE	D	459	152.902	11.230	33.588	1.00	35.98	D

	ATOM	7234	CB	PHE	D	459	151.526	11.848	33.859	1.00	35.38	D
	ATOM	7235	CG	PHE	D	459	151.009	12.705	32.729	1.00	36.52	D
	ATOM	7236	CD1	PHE	D	459	149.643	12.975	32.603	1.00	35.53	D
	ATOM	7237	CD2	PHE	D	459	151.882	13.228	31.773	1.00	36.02	D
5	ATOM	7238	CE1	PHE	D	459	149.160	13.748	31.542	1.00	33.32	D
	ATOM	7239	CE2	PHE	D	459	151.404	13.999	30.715	1.00	34.61	D
	ATOM	7240	CZ	PHE	D	459	150.040	14.258	30.599	1.00	33.14	D
	ATOM	7241	C	PHE	D	459	153.421	10.583	34.858	1.00	35.63	D
	ATOM	7242	O	PHE	D	459	152.927	9.540	35.286	1.00	36.76	D
10	ATOM	7243	N	GLU	D	460	154.436	11.210	35.443	1.00	34.40	D
	ATOM	7244	CA	GLU	D	460	155.042	10.731	36.669	1.00	32.85	D
	ATOM	7245	CB	GLU	D	460	156.541	10.572	36.501	1.00	31.50	D
	ATOM	7246	CG	GLU	D	460	156.912	9.591	35.436	1.00	34.06	D
	ATOM	7247	CD	GLU	D	460	158.340	9.146	35.561	1.00	34.99	D
15	ATOM	7248	OE1	GLU	D	460	159.177	9.996	35.916	1.00	38.06	D
	ATOM	7249	OE2	GLU	D	460	158.634	7.959	35.305	1.00	34.49	D
	ATOM	7250	C	GLU	D	460	154.754	11.770	37.717	1.00	32.81	D
	ATOM	7251	O	GLU	D	460	154.506	12.927	37.387	1.00	33.34	D
	ATOM	7252	N	GLY	D	461	154.788	11.364	38.982	1.00	33.03	D
20	ATOM	7253	CA	GLY	D	461	154.503	12.295	40.057	1.00	31.23	D
	ATOM	7254	C	GLY	D	461	154.150	11.600	41.354	1.00	30.79	D
	ATOM	7255	O	GLY	D	461	154.770	11.857	42.383	1.00	31.55	D
	ATOM	7256	N	HIS	D	462	153.151	10.727	41.318	1.00	30.63	D
	ATOM	7257	CA	HIS	D	462	152.744	10.016	42.522	1.00	30.77	D
25	ATOM	7258	CB	HIS	D	462	151.580	9.065	42.209	1.00	30.12	D
	ATOM	7259	CG	HIS	D	462	150.254	9.754	42.066	1.00	29.59	D
	ATOM	7260	CD2	HIS	D	462	149.387	9.814	41.026	1.00	29.20	D
	ATOM	7261	ND1	HIS	D	462	149.701	10.520	43.070	1.00	27.98	D
	ATOM	7262	CE1	HIS	D	462	148.555	11.027	42.652	1.00	29.48	D
30	ATOM	7263	NE2	HIS	D	462	148.342	10.615	41.415	1.00	29.45	D
	ATOM	7264	C	HIS	D	462	153.935	9.233	43.032	1.00	31.13	D
	ATOM	7265	O	HIS	D	462	154.687	8.672	42.240	1.00	32.76	D
	ATOM	7266	N	ASN	D	463	154.113	9.195	44.349	1.00	31.08	D
	ATOM	7267	CA	ASN	D	463	155.239	8.473	44.929	1.00	30.79	D
35	ATOM	7268	CB	ASN	D	463	155.764	9.212	46.155	1.00	31.33	D
	ATOM	7269	CG	ASN	D	463	156.351	10.572	45.806	1.00	33.80	D
	ATOM	7270	OD1	ASN	D	463	156.669	11.368	46.700	1.00	36.56	D
	ATOM	7271	ND2	ASN	D	463	156.500	10.848	44.511	1.00	31.92	D
	ATOM	7272	C	ASN	D	463	154.863	7.058	45.300	1.00	30.83	D
40	ATOM	7273	O	ASN	D	463	155.678	6.319	45.843	1.00	32.01	D
	ATOM	7274	N	SER	D	464	153.623	6.685	44.996	1.00	30.09	D
	ATOM	7275	CA	SER	D	464	153.099	5.346	45.292	1.00	29.60	D
	ATOM	7276	CB	SER	D	464	152.364	5.358	46.630	1.00	31.07	D
	ATOM	7277	OG	SER	D	464	153.073	4.621	47.611	1.00	34.87	D
45	ATOM	7278	C	SER	D	464	152.125	4.900	44.203	1.00	28.55	D
	ATOM	7279	O	SER	D	464	151.814	5.656	43.289	1.00	29.29	D
	ATOM	7280	N	THR	D	465	151.625	3.676	44.313	1.00	27.12	D
	ATOM	7281	CA	THR	D	465	150.675	3.153	43.331	1.00	25.67	D
	ATOM	7282	CB	THR	D	465	150.036	1.828	43.817	1.00	23.85	D
50	ATOM	7283	OG1	THR	D	465	151.057	0.894	44.197	1.00	24.69	D
	ATOM	7284	CG2	THR	D	465	149.169	1.234	42.742	1.00	22.12	D
	ATOM	7285	C	THR	D	465	149.536	4.150	43.089	1.00	26.17	D
	ATOM	7286	O	THR	D	465	149.122	4.872	44.001	1.00	27.21	D
	ATOM	7287	N	VAL	D	466	149.041	4.197	41.856	1.00	25.63	D

	ATOM	7288	CA	VAL	D	466	147.933	5.078	41.506	1.00	24.45	D
	ATOM	7289	CB	VAL	D	466	148.003	5.484	39.994	1.00	26.90	D
	ATOM	7290	CG1	VAL	D	466	146.795	6.351	39.597	1.00	27.11	D
	ATOM	7291	CG2	VAL	D	466	149.300	6.240	39.732	1.00	27.75	D
5	ATOM	7292	C	VAL	D	466	146.740	4.165	41.783	1.00	22.49	D
	ATOM	7293	O	VAL	D	466	146.604	3.130	41.148	1.00	19.72	D
	ATOM	7294	N	ARG	D	467	145.894	4.543	42.737	1.00	21.80	D
	ATOM	7295	CA	ARG	D	467	144.764	3.713	43.121	1.00	21.09	D
	ATOM	7296	CB	ARG	D	467	144.529	3.828	44.637	1.00	21.63	D
10	ATOM	7297	CG	ARG	D	467	143.582	2.778	45.221	1.00	24.03	D
	ATOM	7298	CD	ARG	D	467	144.190	1.398	45.033	1.00	25.89	D
	ATOM	7299	NE	ARG	D	467	143.247	0.294	45.158	1.00	27.91	D
	ATOM	7300	CZ	ARG	D	467	142.283	0.013	44.288	1.00	30.10	D
	ATOM	7301	NH1	ARG	D	467	142.117	0.776	43.214	1.00	32.22	D
15	ATOM	7302	NH2	ARG	D	467	141.515	-1.064	44.469	1.00	28.51	D
	ATOM	7303	C	ARG	D	467	143.463	3.984	42.370	1.00	21.53	D
	ATOM	7304	O	ARG	D	467	142.666	3.071	42.152	1.00	21.18	D
	ATOM	7305	N	CYS	D	468	143.240	5.225	41.960	1.00	21.08	D
	ATOM	7306	CA	CYS	D	468	142.008	5.538	41.259	1.00	22.04	D
20	ATOM	7307	CB	CYS	D	468	140.874	5.672	42.282	1.00	22.73	D
	ATOM	7308	SG	CYS	D	468	141.036	7.052	43.480	1.00	26.78	D
	ATOM	7309	C	CYS	D	468	142.141	6.807	40.433	1.00	22.89	D
	ATOM	7310	O	CYS	D	468	143.034	7.617	40.672	1.00	24.06	D
	ATOM	7311	N	LEU	D	469	141.247	6.995	39.466	1.00	23.65	D
25	ATOM	7312	CA	LEU	D	469	141.321	8.189	38.614	1.00	25.22	D
	ATOM	7313	CB	LEU	D	469	142.382	7.997	37.512	1.00	25.67	D
	ATOM	7314	CG	LEU	D	469	142.191	6.914	36.441	1.00	25.46	D
	ATOM	7315	CD1	LEU	D	469	140.965	7.170	35.605	1.00	24.47	D
	ATOM	7316	CD2	LEU	D	469	143.428	6.891	35.560	1.00	26.81	D
30	ATOM	7317	C	LEU	D	469	140.005	8.574	37.960	1.00	24.60	D
	ATOM	7318	O	LEU	D	469	139.162	7.729	37.690	1.00	24.12	D
	ATOM	7319	N	ASP	D	470	139.818	9.853	37.693	1.00	24.30	D
	ATOM	7320	CA	ASP	D	470	138.584	10.242	37.043	1.00	24.73	D
	ATOM	7321	CB	ASP	D	470	137.540	10.594	38.118	1.00	24.80	D
35	ATOM	7322	CG	ASP	D	470	136.109	10.685	37.571	1.00	24.84	D
	ATOM	7323	OD1	ASP	D	470	135.842	10.240	36.441	1.00	25.89	D
	ATOM	7324	OD2	ASP	D	470	135.242	11.197	38.296	1.00	23.60	D
	ATOM	7325	C	ASP	D	470	138.857	11.409	36.091	1.00	24.57	D
	ATOM	7326	O	ASP	D	470	139.863	12.118	36.214	1.00	23.14	D
40	ATOM	7327	N	ILE	D	471	137.988	11.584	35.110	1.00	24.45	D
	ATOM	7328	CA	ILE	D	471	138.184	12.684	34.197	1.00	26.31	D
	ATOM	7329	CB	ILE	D	471	138.389	12.210	32.737	1.00	24.06	D
	ATOM	7330	CG2	ILE	D	471	138.861	13.393	31.915	1.00	24.13	D
	ATOM	7331	CG1	ILE	D	471	139.454	11.097	32.656	1.00	22.43	D
45	ATOM	7332	CD1	ILE	D	471	139.553	10.449	31.293	1.00	18.18	D
	ATOM	7333	C	ILE	D	471	136.971	13.600	34.271	1.00	28.56	D
	ATOM	7334	O	ILE	D	471	135.833	13.135	34.280	1.00	30.74	D
	ATOM	7335	N	VAL	D	472	137.222	14.901	34.358	1.00	30.47	D
	ATOM	7336	CA	VAL	D	472	136.157	15.892	34.433	1.00	31.86	D
50	ATOM	7337	CB	VAL	D	472	136.105	16.544	35.857	1.00	31.83	D
	ATOM	7338	CG1	VAL	D	472	135.793	15.474	36.896	1.00	30.28	D
	ATOM	7339	CG2	VAL	D	472	137.427	17.231	36.193	1.00	27.41	D
	ATOM	7340	C	VAL	D	472	136.369	16.966	33.358	1.00	33.87	D
	ATOM	7341	O	VAL	D	472	137.474	17.119	32.826	1.00	34.57	D

	ATOM	7342	N	GLU	D	473	135.304	17.692	33.026	1.00	35.69	D
	ATOM	7343	CA	GLU	D	473	135.354	18.747	32.004	1.00	37.97	D
	ATOM	7344	CB	GLU	D	473	134.565	18.321	30.751	1.00	39.26	D
	ATOM	7345	CG	GLU	D	473	134.587	19.326	29.567	1.00	41.82	D
5	ATOM	7346	CD	GLU	D	473	133.581	18.966	28.455	1.00	41.92	D
	ATOM	7347	OE1	GLU	D	473	133.651	17.853	27.893	1.00	41.68	D
	ATOM	7348	OE2	GLU	D	473	132.712	19.801	28.145	1.00	42.75	D
	ATOM	7349	C	GLU	D	473	134.722	19.983	32.620	1.00	38.63	D
	ATOM	7350	O	GLU	D	473	133.585	19.944	33.084	1.00	39.66	D
10	ATOM	7351	N	TYR	D	474	135.464	21.077	32.651	1.00	39.16	D
	ATOM	7352	CA	TYR	D	474	134.952	22.311	33.231	1.00	39.98	D
	ATOM	7353	CB	TYR	D	474	135.534	22.496	34.630	1.00	39.54	D
	ATOM	7354	CG	TYR	D	474	135.126	23.777	35.311	1.00	40.62	D
	ATOM	7355	CD1	TYR	D	474	133.802	24.002	35.686	1.00	40.93	D
15	ATOM	7356	CE1	TYR	D	474	133.432	25.174	36.332	1.00	40.40	D
	ATOM	7357	CD2	TYR	D	474	136.072	24.761	35.601	1.00	40.52	D
	ATOM	7358	CE2	TYR	D	474	135.714	25.933	36.243	1.00	40.34	D
	ATOM	7359	CZ	TYR	D	474	134.393	26.134	36.604	1.00	40.71	D
	ATOM	7360	OH	TYR	D	474	134.025	27.300	37.224	1.00	41.79	D
20	ATOM	7361	C	TYR	D	474	135.422	23.394	32.277	1.00	39.99	D
	ATOM	7362	O	TYR	D	474	136.550	23.339	31.784	1.00	40.02	D
	ATOM	7363	N	LYS	D	475	134.551	24.357	31.998	1.00	40.09	D
	ATOM	7364	CA	LYS	D	475	134.868	25.438	31.069	1.00	42.55	D
	ATOM	7365	CB	LYS	D	475	135.796	26.471	31.723	1.00	43.10	D
25	ATOM	7366	CG	LYS	D	475	135.185	27.292	32.864	1.00	43.55	D
	ATOM	7367	CD	LYS	D	475	136.276	28.148	33.502	1.00	46.85	D
	ATOM	7368	CE	LYS	D	475	135.765	29.052	34.623	1.00	48.93	D
	ATOM	7369	NZ	LYS	D	475	134.765	30.077	34.181	1.00	49.55	D
	ATOM	7370	C	LYS	D	475	135.529	24.888	29.804	1.00	43.23	D
30	ATOM	7371	O	LYS	D	475	136.556	25.401	29.352	1.00	43.08	D
	ATOM	7372	N	ASN	D	476	134.943	23.831	29.248	1.00	44.27	D
	ATOM	7373	CA	ASN	D	476	135.449	23.202	28.024	1.00	44.54	D
	ATOM	7374	CB	ASN	D	476	135.383	24.180	26.850	1.00	44.94	D
	ATOM	7375	CG	ASN	D	476	134.054	24.135	26.140	1.00	44.85	D
35	ATOM	7376	OD1	ASN	D	476	133.040	24.596	26.665	1.00	44.09	D
	ATOM	7377	ND2	ASN	D	476	134.048	23.565	24.934	1.00	45.89	D
	ATOM	7378	C	ASN	D	476	136.841	22.591	28.077	1.00	44.03	D
	ATOM	7379	O	ASN	D	476	137.403	22.230	27.036	1.00	44.45	D
	ATOM	7380	N	ILE	D	477	137.400	22.474	29.280	1.00	43.98	D
40	ATOM	7381	CA	ILE	D	477	138.722	21.860	29.459	1.00	42.39	D
	ATOM	7382	CB	ILE	D	477	139.681	22.744	30.260	1.00	42.82	D
	ATOM	7383	CG2	ILE	D	477	141.024	22.052	30.387	1.00	43.06	D
	ATOM	7384	CG1	ILE	D	477	139.842	24.097	29.583	1.00	42.36	D
	ATOM	7385	CD1	ILE	D	477	140.465	25.135	30.486	1.00	41.94	D
45	ATOM	7386	C	ILE	D	477	138.528	20.578	30.249	1.00	41.19	D
	ATOM	7387	O	ILE	D	477	137.805	20.560	31.253	1.00	40.43	D
	ATOM	7388	N	LYS	D	478	139.166	19.511	29.777	1.00	38.84	D
	ATOM	7389	CA	LYS	D	478	139.078	18.212	30.428	1.00	36.96	D
	ATOM	7390	CB	LYS	D	478	139.070	17.085	29.394	1.00	35.75	D
50	ATOM	7391	CG	LYS	D	478	137.740	16.932	28.687	1.00	35.23	D
	ATOM	7392	CD	LYS	D	478	137.557	15.519	28.160	1.00	32.30	D
	ATOM	7393	CE	LYS	D	478	136.120	15.312	27.725	1.00	31.88	D
	ATOM	7394	NZ	LYS	D	478	135.743	13.871	27.552	1.00	32.71	D
	ATOM	7395	C	LYS	D	478	140.218	17.984	31.402	1.00	36.46	D

	ATOM	7396	O	LYS	D	478	141.381	18.009	31.015	1.00	36.77	D
	ATOM	7397	N	TYR	D	479	139.884	17.749	32.666	1.00	35.14	D
	ATOM	7398	CA	TYR	D	479	140.906	17.514	33.675	1.00	34.37	D
	ATOM	7399	CB	TYR	D	479	140.674	18.442	34.875	1.00	33.93	D
5	ATOM	7400	CG	TYR	D	479	140.847	19.914	34.543	1.00	34.98	D
	ATOM	7401	CD1	TYR	D	479	142.108	20.529	34.614	1.00	33.05	D
	ATOM	7402	CE1	TYR	D	479	142.264	21.880	34.300	1.00	32.76	D
	ATOM	7403	CD2	TYR	D	479	139.753	20.691	34.147	1.00	33.92	D
	ATOM	7404	CE2	TYR	D	479	139.901	22.037	33.830	1.00	34.11	D
10	ATOM	7405	CZ	TYR	D	479	141.152	22.624	33.907	1.00	34.22	D
	ATOM	7406	OH	TYR	D	479	141.270	23.952	33.573	1.00	37.80	D
	ATOM	7407	C	TYR	D	479	140.936	16.061	34.134	1.00	32.92	D
	ATOM	7408	O	TYR	D	479	139.903	15.404	34.218	1.00	32.94	D
	ATOM	7409	N	ILE	D	480	142.138	15.569	34.412	1.00	31.23	D
15	ATOM	7410	CA	ILE	D	480	142.344	14.213	34.910	1.00	30.00	D
	ATOM	7411	CB	ILE	D	480	143.568	13.528	34.236	1.00	30.27	D
	ATOM	7412	CG2	ILE	D	480	143.826	12.150	34.879	1.00	31.07	D
	ATOM	7413	CG1	ILE	D	480	143.335	13.334	32.741	1.00	31.12	D
	ATOM	7414	CD1	ILE	D	480	144.440	12.531	32.060	1.00	26.66	D
20	ATOM	7415	C	ILE	D	480	142.674	14.314	36.417	1.00	29.96	D
	ATOM	7416	O	ILE	D	480	143.583	15.063	36.808	1.00	29.34	D
	ATOM	7417	N	VAL	D	481	141.944	13.582	37.263	1.00	28.07	D
	ATOM	7418	CA	VAL	D	481	142.234	13.590	38.702	1.00	26.17	D
	ATOM	7419	CB	VAL	D	481	141.048	14.099	39.550	1.00	25.50	D
25	ATOM	7420	CG1	VAL	D	481	141.533	14.438	40.943	1.00	25.80	D
	ATOM	7421	CG2	VAL	D	481	140.431	15.338	38.910	1.00	26.04	D
	ATOM	7422	C	VAL	D	481	142.587	12.166	39.110	1.00	26.07	D
	ATOM	7423	O	VAL	D	481	141.848	11.232	38.812	1.00	26.50	D
	ATOM	7424	N	THR	D	482	143.734	12.006	39.766	1.00	26.06	D
30	ATOM	7425	CA	THR	D	482	144.217	10.691	40.184	1.00	26.60	D
	ATOM	7426	CB	THR	D	482	145.520	10.324	39.440	1.00	25.75	D
	ATOM	7427	OG1	THR	D	482	146.452	11.402	39.568	1.00	23.78	D
	ATOM	7428	CG2	THR	D	482	145.252	10.057	37.971	1.00	26.32	D
	ATOM	7429	C	THR	D	482	144.496	10.591	41.688	1.00	27.46	D
35	ATOM	7430	O	THR	D	482	145.180	11.444	42.267	1.00	29.29	D
	ATOM	7431	N	GLY	D	483	143.977	9.530	42.303	1.00	25.97	D
	ATOM	7432	CA	GLY	D	483	144.176	9.303	43.724	1.00	24.32	D
	ATOM	7433	C	GLY	D	483	145.201	8.206	43.922	1.00	23.49	D
	ATOM	7434	O	GLY	D	483	145.156	7.171	43.236	1.00	23.98	D
40	ATOM	7435	N	SER	D	484	146.106	8.428	44.877	1.00	22.04	D
	ATOM	7436	CA	SER	D	484	147.208	7.503	45.153	1.00	21.89	D
	ATOM	7437	CB	SER	D	484	148.540	8.193	44.820	1.00	19.14	D
	ATOM	7438	OG	SER	D	484	149.640	7.324	45.038	1.00	17.25	D
	ATOM	7439	C	SER	D	484	147.266	7.012	46.582	1.00	22.62	D
45	ATOM	7440	O	SER	D	484	146.488	7.433	47.426	1.00	25.82	D
	ATOM	7441	N	ARG	D	485	148.193	6.100	46.837	1.00	24.32	D
	ATOM	7442	CA	ARG	D	485	148.412	5.585	48.179	1.00	26.12	D
	ATOM	7443	CB	ARG	D	485	149.052	4.206	48.134	1.00	27.36	D
	ATOM	7444	CG	ARG	D	485	148.168	3.160	47.556	1.00	28.76	D
50	ATOM	7445	CD	ARG	D	485	148.786	1.809	47.722	1.00	29.11	D
	ATOM	7446	NE	ARG	D	485	147.768	0.784	47.543	1.00	31.30	D
	ATOM	7447	CZ	ARG	D	485	148.031	-0.500	47.350	1.00	31.33	D
	ATOM	7448	NH1	ARG	D	485	149.283	-0.931	47.304	1.00	30.94	D
	ATOM	7449	NH2	ARG	D	485	147.039	-1.353	47.214	1.00	31.96	D

	ATOM	7450	C	ARG	D	485	149.367	6.534	48.886	1.00	27.46	D
	ATOM	7451	O	ARG	D	485	149.712	6.329	50.045	1.00	28.74	D
	ATOM	7452	N	ASP	D	486	149.822	7.561	48.186	1.00	27.88	D
	ATOM	7453	CA	ASP	D	486	150.722	8.487	48.819	1.00	27.38	D
5	ATOM	7454	CB	ASP	D	486	151.631	9.137	47.789	1.00	29.39	D
	ATOM	7455	CG	ASP	D	486	150.858	9.822	46.695	1.00	30.30	D
	ATOM	7456	OD1	ASP	D	486	149.693	10.190	46.951	1.00	28.83	D
	ATOM	7457	OD2	ASP	D	486	151.410	10.006	45.591	1.00	33.15	D
	ATOM	7458	C	ASP	D	486	149.947	9.547	49.566	1.00	26.08	D
10	ATOM	7459	O	ASP	D	486	150.524	10.533	49.997	1.00	26.51	D
	ATOM	7460	N	ASN	D	487	148.643	9.343	49.727	1.00	26.47	D
	ATOM	7461	CA	ASN	D	487	147.778	10.295	50.449	1.00	28.03	D
	ATOM	7462	CB	ASN	D	487	148.466	10.859	51.720	1.00	24.22	D
	ATOM	7463	CG	ASN	D	487	149.130	9.783	52.608	1.00	25.85	D
15	ATOM	7464	OD1	ASN	D	487	150.077	10.094	53.357	1.00	25.75	D
	ATOM	7465	ND2	ASN	D	487	148.639	8.536	52.543	1.00	23.88	D
	ATOM	7466	C	ASN	D	487	147.331	11.492	49.578	1.00	29.17	D
	ATOM	7467	O	ASN	D	487	146.419	12.233	49.958	1.00	30.88	D
	ATOM	7468	N	THR	D	488	147.959	11.686	48.419	1.00	30.51	D
20	ATOM	7469	CA	THR	D	488	147.599	12.817	47.574	1.00	31.76	D
	ATOM	7470	CB	THR	D	488	148.867	13.590	47.044	1.00	32.19	D
	ATOM	7471	OG1	THR	D	488	149.361	12.984	45.841	1.00	30.87	D
	ATOM	7472	CG2	THR	D	488	149.968	13.586	48.078	1.00	32.86	D
	ATOM	7473	C	THR	D	488	146.708	12.444	46.387	1.00	33.20	D
25	ATOM	7474	O	THR	D	488	146.374	11.267	46.172	1.00	32.98	D
	ATOM	7475	N	LEU	D	489	146.310	13.480	45.650	1.00	34.03	D
	ATOM	7476	CA	LEU	D	489	145.468	13.377	44.465	1.00	34.19	D
	ATOM	7477	CB	LEU	D	489	144.056	13.869	44.779	1.00	34.15	D
	ATOM	7478	CG	LEU	D	489	143.138	12.961	45.589	1.00	34.12	D
30	ATOM	7479	CD1	LEU	D	489	142.459	13.747	46.710	1.00	33.50	D
	ATOM	7480	CD2	LEU	D	489	142.102	12.369	44.642	1.00	32.16	D
	ATOM	7481	C	LEU	D	489	146.084	14.320	43.448	1.00	33.40	D
	ATOM	7482	O	LEU	D	489	145.854	15.519	43.533	1.00	34.39	D
	ATOM	7483	N	HIS	D	490	146.876	13.818	42.506	1.00	32.48	D
35	ATOM	7484	CA	HIS	D	490	147.465	14.727	41.522	1.00	31.60	D
	ATOM	7485	CB	HIS	D	490	148.744	14.136	40.909	1.00	31.07	D
	ATOM	7486	CG	HIS	D	490	149.914	14.125	41.846	1.00	31.65	D
	ATOM	7487	CD2	HIS	D	490	149.977	14.042	43.197	1.00	32.29	D
	ATOM	7488	ND1	HIS	D	490	151.219	14.191	41.407	1.00	33.73	D
40	ATOM	7489	CE1	HIS	D	490	152.036	14.152	42.446	1.00	33.37	D
	ATOM	7490	NE2	HIS	D	490	151.306	14.061	43.543	1.00	32.68	D
	ATOM	7491	C	HIS	D	490	146.456	15.034	40.429	1.00	30.39	D
	ATOM	7492	O	HIS	D	490	145.735	14.149	39.983	1.00	31.27	D
	ATOM	7493	N	VAL	D	491	146.391	16.296	40.022	1.00	29.80	D
45	ATOM	7494	CA	VAL	D	491	145.466	16.726	38.977	1.00	31.12	D
	ATOM	7495	CB	VAL	D	491	144.610	17.941	39.472	1.00	30.67	D
	ATOM	7496	CG1	VAL	D	491	143.683	18.442	38.365	1.00	29.26	D
	ATOM	7497	CG2	VAL	D	491	143.798	17.544	40.683	1.00	29.19	D
	ATOM	7498	C	VAL	D	491	146.256	17.127	37.712	1.00	32.27	D
50	ATOM	7499	O	VAL	D	491	147.249	17.850	37.802	1.00	33.21	D
	ATOM	7500	N	TRP	D	492	145.829	16.647	36.545	1.00	32.46	D
	ATOM	7501	CA	TRP	D	492	146.501	16.975	35.285	1.00	33.55	D
	ATOM	7502	CB	TRP	D	492	147.308	15.798	34.759	1.00	33.18	D
	ATOM	7503	CG	TRP	D	492	147.697	14.828	35.788	1.00	34.51	D

	ATOM	7504	CD2	TRP	D	492	149.014	14.604	36.288	1.00	35.06	D
	ATOM	7505	CE2	TRP	D	492	148.930	13.552	37.224	1.00	34.88	D
	ATOM	7506	CE3	TRP	D	492	150.263	15.189	36.034	1.00	33.09	D
	ATOM	7507	CD1	TRP	D	492	146.884	13.936	36.423	1.00	34.18	D
5	ATOM	7508	NE1	TRP	D	492	147.617	13.161	37.285	1.00	34.58	D
	ATOM	7509	CZ2	TRP	D	492	150.048	13.073	37.906	1.00	34.36	D
	ATOM	7510	CZ3	TRP	D	492	151.371	14.715	36.710	1.00	32.50	D
	ATOM	7511	CH2	TRP	D	492	151.258	13.667	37.634	1.00	33.38	D
	ATOM	7512	C	TRP	D	492	145.475	17.318	34.226	1.00	34.32	D
10	ATOM	7513	O	TRP	D	492	144.338	16.864	34.292	1.00	35.53	D
	ATOM	7514	N	LYS	D	493	145.859	18.110	33.236	1.00	34.28	D
	ATOM	7515	CA	LYS	D	493	144.900	18.433	32.202	1.00	35.06	D
	ATOM	7516	CB	LYS	D	493	145.116	19.860	31.694	1.00	35.38	D
	ATOM	7517	CG	LYS	D	493	146.531	20.133	31.281	1.00	37.78	D
15	ATOM	7518	CD	LYS	D	493	146.739	21.563	30.810	1.00	39.13	D
	ATOM	7519	CE	LYS	D	493	146.643	22.588	31.928	1.00	37.56	D
	ATOM	7520	NZ	LYS	D	493	147.094	23.906	31.410	1.00	35.80	D
	ATOM	7521	C	LYS	D	493	145.075	17.408	31.084	1.00	34.97	D
	ATOM	7522	O	LYS	D	493	146.182	17.192	30.600	1.00	33.77	D
20	ATOM	7523	N	LEU	D	494	143.981	16.753	30.706	1.00	36.70	D
	ATOM	7524	CA	LEU	D	494	144.018	15.744	29.659	1.00	39.45	D
	ATOM	7525	CB	LEU	D	494	142.630	15.126	29.458	1.00	39.18	D
	ATOM	7526	CG	LEU	D	494	142.458	14.046	28.380	1.00	38.09	D
	ATOM	7527	CD1	LEU	D	494	143.506	12.972	28.552	1.00	36.77	D
25	ATOM	7528	CD2	LEU	D	494	141.043	13.442	28.448	1.00	36.96	D
	ATOM	7529	C	LEU	D	494	144.493	16.382	28.366	1.00	42.52	D
	ATOM	7530	O	LEU	D	494	143.928	17.387	27.912	1.00	42.98	D
	ATOM	7531	N	PRO	D	495	145.559	15.819	27.764	1.00	45.09	D
	ATOM	7532	CD	PRO	D	495	146.315	14.686	28.330	1.00	45.01	D
30	ATOM	7533	CA	PRO	D	495	146.168	16.287	26.505	1.00	45.59	D
	ATOM	7534	CB	PRO	D	495	147.255	15.253	26.241	1.00	45.10	D
	ATOM	7535	CG	PRO	D	495	147.633	14.802	27.619	1.00	45.87	D
	ATOM	7536	C	PRO	D	495	145.146	16.324	25.365	1.00	46.50	D
	ATOM	7537	O	PRO	D	495	144.334	15.409	25.243	1.00	47.18	D
35	ATOM	7538	N	LYS	D	496	145.194	17.360	24.525	1.00	47.14	D
	ATOM	7539	CA	LYS	D	496	144.254	17.491	23.400	1.00	47.35	D
	ATOM	7540	CB	LYS	D	496	143.768	18.942	23.268	1.00	47.30	D
	ATOM	7541	CG	LYS	D	496	143.109	19.501	24.520	0.00	47.88	D
	ATOM	7542	CD	LYS	D	496	141.811	18.778	24.840	0.00	48.23	D
40	ATOM	7543	CE	LYS	D	496	141.133	19.370	26.065	0.00	48.50	D
	ATOM	7544	NZ	LYS	D	496	139.817	18.722	26.331	0.00	48.74	D
	ATOM	7545	C	LYS	D	496	144.853	17.046	22.064	1.00	47.41	D
	ATOM	7546	O	LYS	D	496	145.277	15.898	21.895	1.00	46.92	D
	ATOM	7547	N	ASP	D	508	157.546	8.144	18.136	1.00	82.08	D
45	ATOM	7548	CA	ASP	D	508	158.190	8.937	19.182	1.00	81.66	D
	ATOM	7549	CB	ASP	D	508	158.981	10.090	18.569	1.00	82.86	D
	ATOM	7550	CG	ASP	D	508	158.086	11.249	18.168	1.00	83.90	D
	ATOM	7551	OD1	ASP	D	508	157.135	11.025	17.381	1.00	83.92	D
	ATOM	7552	OD2	ASP	D	508	158.334	12.378	18.644	1.00	83.63	D
50	ATOM	7553	C	ASP	D	508	157.121	9.528	20.096	1.00	80.44	D
	ATOM	7554	O	ASP	D	508	157.419	10.346	20.972	1.00	80.05	D
	ATOM	7555	N	TYR	D	509	155.874	9.120	19.884	1.00	78.72	D
	ATOM	7556	CA	TYR	D	509	154.768	9.631	20.678	1.00	76.03	D
	ATOM	7557	CB	TYR	D	509	153.454	8.997	20.254	1.00	76.05	D

	ATOM	7558	CG	TYR	D	509	152.443	10.025	19.841	1.00	77.13	D
	ATOM	7559	CD1	TYR	D	509	152.268	11.195	20.579	1.00	77.84	D
	ATOM	7560	CE1	TYR	D	509	151.324	12.147	20.205	1.00	79.73	D
	ATOM	7561	CD2	TYR	D	509	151.653	9.830	18.719	1.00	78.10	D
5	ATOM	7562	CE2	TYR	D	509	150.709	10.769	18.335	1.00	79.97	D
	ATOM	7563	CZ	TYR	D	509	150.543	11.923	19.080	1.00	80.67	D
	ATOM	7564	OH	TYR	D	509	149.570	12.832	18.715	1.00	82.17	D
	ATOM	7565	C	TYR	D	509	154.938	9.440	22.170	1.00	73.80	D
	ATOM	7566	O	TYR	D	509	154.457	10.253	22.960	1.00	75.57	D
10	ATOM	7567	N	PRO	D	510	155.602	8.352	22.588	1.00	70.29	D
	ATOM	7568	CD	PRO	D	510	156.084	7.160	21.860	1.00	68.38	D
	ATOM	7569	CA	PRO	D	510	155.758	8.194	24.039	1.00	66.01	D
	ATOM	7570	CB	PRO	D	510	156.600	6.929	24.150	1.00	66.48	D
	ATOM	7571	CG	PRO	D	510	156.132	6.128	22.949	1.00	68.27	D
15	ATOM	7572	C	PRO	D	510	156.446	9.424	24.644	1.00	62.34	D
	ATOM	7573	O	PRO	D	510	157.667	9.504	24.676	1.00	62.17	D
	ATOM	7574	N	LEU	D	511	155.655	10.392	25.096	1.00	58.50	D
	ATOM	7575	CA	LEU	D	511	156.197	11.603	25.700	1.00	54.92	D
	ATOM	7576	CB	LEU	D	511	155.354	12.806	25.313	1.00	54.10	D
20	ATOM	7577	CG	LEU	D	511	155.130	12.940	23.807	1.00	52.83	D
	ATOM	7578	CD1	LEU	D	511	154.228	14.114	23.521	1.00	51.33	D
	ATOM	7579	CD2	LEU	D	511	156.467	13.102	23.107	1.00	52.54	D
	ATOM	7580	C	LEU	D	511	156.188	11.451	27.211	1.00	53.49	D
	ATOM	7581	O	LEU	D	511	155.145	11.576	27.847	1.00	53.00	D
25	ATOM	7582	N	VAL	D	512	157.359	11.184	27.778	1.00	52.14	D
	ATOM	7583	CA	VAL	D	512	157.506	10.992	29.213	1.00	49.88	D
	ATOM	7584	CB	VAL	D	512	158.576	9.937	29.498	1.00	48.71	D
	ATOM	7585	CG1	VAL	D	512	158.654	9.664	30.992	1.00	49.81	D
	ATOM	7586	CG2	VAL	D	512	158.262	8.666	28.725	1.00	47.64	D
30	ATOM	7587	C	VAL	D	512	157.889	12.265	29.954	1.00	49.28	D
	ATOM	7588	O	VAL	D	512	158.855	12.925	29.592	1.00	48.19	D
	ATOM	7589	N	PHE	D	513	157.126	12.598	30.994	1.00	50.24	D
	ATOM	7590	CA	PHE	D	513	157.397	13.778	31.823	1.00	51.82	D
	ATOM	7591	CB	PHE	D	513	156.158	14.671	31.950	1.00	51.83	D
35	ATOM	7592	CG	PHE	D	513	155.565	15.091	30.632	1.00	52.04	D
	ATOM	7593	CD1	PHE	D	513	154.849	14.187	29.856	1.00	52.52	D
	ATOM	7594	CD2	PHE	D	513	155.724	16.392	30.164	1.00	51.87	D
	ATOM	7595	CE1	PHE	D	513	154.305	14.571	28.635	1.00	52.41	D
	ATOM	7596	CE2	PHE	D	513	155.182	16.785	28.944	1.00	51.44	D
40	ATOM	7597	CZ	PHE	D	513	154.472	15.873	28.181	1.00	51.72	D
	ATOM	7598	C	PHE	D	513	157.807	13.318	33.225	1.00	52.58	D
	ATOM	7599	O	PHE	D	513	156.957	13.164	34.100	1.00	53.73	D
	ATOM	7600	N	HIS	D	514	159.107	13.108	33.427	1.00	52.88	D
	ATOM	7601	CA	HIS	D	514	159.649	12.656	34.707	1.00	52.63	D
45	ATOM	7602	CB	HIS	D	514	161.150	12.425	34.577	1.00	52.45	D
	ATOM	7603	CG	HIS	D	514	161.495	11.297	33.662	1.00	53.43	D
	ATOM	7604	CD2	HIS	D	514	161.857	11.285	32.358	1.00	53.76	D
	ATOM	7605	ND1	HIS	D	514	161.411	9.977	34.049	1.00	54.13	D
	ATOM	7606	CE1	HIS	D	514	161.705	9.199	33.023	1.00	54.22	D
50	ATOM	7607	NE2	HIS	D	514	161.979	9.968	31.985	1.00	55.05	D
	ATOM	7608	C	HIS	D	514	159.388	13.615	35.855	1.00	53.18	D
	ATOM	7609	O	HIS	D	514	159.096	13.204	36.986	1.00	54.06	D
	ATOM	7610	N	THR	D	515	159.494	14.901	35.569	1.00	52.64	D
	ATOM	7611	CA	THR	D	515	159.281	15.888	36.597	1.00	52.40	D

	ATOM	7612	CB	THR	D	515	160.524	16.788	36.742	1.00	52.48	D
	ATOM	7613	OG1	THR	D	515	160.166	17.996	37.420	1.00	52.59	D
	ATOM	7614	CG2	THR	D	515	161.126	17.093	35.381	1.00	52.87	D
	ATOM	7615	C	THR	D	515	158.029	16.705	36.322	1.00	52.17	D
5	ATOM	7616	O	THR	D	515	157.858	17.269	35.245	1.00	51.18	D
	ATOM	7617	N	PRO	D	516	157.114	16.736	37.304	1.00	53.39	D
	ATOM	7618	CD	PRO	D	516	157.164	15.841	38.478	1.00	53.89	D
	ATOM	7619	CA	PRO	D	516	155.835	17.449	37.271	1.00	52.84	D
	ATOM	7620	CB	PRO	D	516	155.231	17.119	38.632	1.00	52.59	D
10	ATOM	7621	CG	PRO	D	516	155.703	15.729	38.851	1.00	52.83	D
	ATOM	7622	C	PRO	D	516	155.976	18.939	37.057	1.00	51.67	D
	ATOM	7623	O	PRO	D	516	155.238	19.533	36.279	1.00	52.06	D
	ATOM	7624	N	GLU	D	517	156.925	19.545	37.751	1.00	51.53	D
	ATOM	7625	CA	GLU	D	517	157.115	20.974	37.615	1.00	51.30	D
15	ATOM	7626	CB	GLU	D	517	158.171	21.456	38.611	1.00	53.01	D
	ATOM	7627	CG	GLU	D	517	157.783	21.225	40.076	1.00	55.65	D
	ATOM	7628	CD	GLU	D	517	156.339	21.648	40.384	1.00	57.61	D
	ATOM	7629	OE1	GLU	D	517	155.899	22.718	39.901	1.00	58.27	D
	ATOM	7630	OE2	GLU	D	517	155.641	20.911	41.115	1.00	58.41	D
20	ATOM	7631	C	GLU	D	517	157.482	21.376	36.180	1.00	50.73	D
	ATOM	7632	O	GLU	D	517	157.417	22.549	35.824	1.00	50.38	D
	ATOM	7633	N	GLU	D	518	157.853	20.408	35.350	1.00	49.94	D
	ATOM	7634	CA	GLU	D	518	158.200	20.707	33.964	1.00	48.95	D
	ATOM	7635	CB	GLU	D	518	159.552	20.081	33.613	1.00	49.87	D
25	ATOM	7636	CG	GLU	D	518	160.741	20.801	34.239	1.00	51.31	D
	ATOM	7637	CD	GLU	D	518	162.074	20.125	33.945	1.00	52.52	D
	ATOM	7638	OE1	GLU	D	518	162.225	19.579	32.823	1.00	53.98	D
	ATOM	7639	OE2	GLU	D	518	162.971	20.153	34.826	1.00	50.01	D
	ATOM	7640	C	GLU	D	518	157.119	20.209	33.003	1.00	47.92	D
30	ATOM	7641	O	GLU	D	518	157.143	20.496	31.808	1.00	47.01	D
	ATOM	7642	N	ASN	D	519	156.164	19.465	33.541	1.00	47.59	D
	ATOM	7643	CA	ASN	D	519	155.071	18.933	32.746	1.00	46.99	D
	ATOM	7644	CB	ASN	D	519	154.490	17.710	33.459	1.00	45.93	D
	ATOM	7645	CG	ASN	D	519	153.454	16.995	32.633	1.00	45.28	D
35	ATOM	7646	OD1	ASN	D	519	152.907	15.970	33.055	1.00	45.38	D
	ATOM	7647	ND2	ASN	D	519	153.173	17.526	31.445	1.00	42.56	D
	ATOM	7648	C	ASN	D	519	153.998	20.023	32.551	1.00	46.69	D
	ATOM	7649	O	ASN	D	519	153.408	20.516	33.524	1.00	46.92	D
	ATOM	7650	N	PRO	D	520	153.758	20.431	31.291	1.00	45.28	D
40	ATOM	7651	CD	PRO	D	520	154.544	20.037	30.110	1.00	43.44	D
	ATOM	7652	CA	PRO	D	520	152.769	21.460	30.937	1.00	44.93	D
	ATOM	7653	CB	PRO	D	520	152.965	21.621	29.431	1.00	43.10	D
	ATOM	7654	CG	PRO	D	520	154.396	21.232	29.234	1.00	43.83	D
	ATOM	7655	C	PRO	D	520	151.328	21.058	31.265	1.00	44.42	D
45	ATOM	7656	O	PRO	D	520	150.430	21.899	31.341	1.00	45.05	D
	ATOM	7657	N	TYR	D	521	151.126	19.764	31.465	1.00	43.22	D
	ATOM	7658	CA	TYR	D	521	149.808	19.216	31.733	1.00	42.86	D
	ATOM	7659	CB	TYR	D	521	149.707	17.885	31.017	1.00	42.46	D
	ATOM	7660	CG	TYR	D	521	150.006	17.994	29.543	1.00	41.84	D
50	ATOM	7661	CD1	TYR	D	521	149.117	18.639	28.684	1.00	43.00	D
	ATOM	7662	CE1	TYR	D	521	149.330	18.673	27.315	1.00	42.26	D
	ATOM	7663	CD2	TYR	D	521	151.135	17.395	28.996	1.00	42.03	D
	ATOM	7664	CE2	TYR	D	521	151.363	17.422	27.625	1.00	42.28	D
	ATOM	7665	CZ	TYR	D	521	150.445	18.058	26.788	1.00	43.30	D

	ATOM	7666	OH	TYR	D	521	150.592	18.015	25.418	1.00	44.00	D
	ATOM	7667	C	TYR	D	521	149.444	19.047	33.211	1.00	42.72	D
	ATOM	7668	O	TYR	D	521	148.267	18.922	33.567	1.00	42.06	D
	ATOM	7669	N	PHE	D	522	150.459	19.030	34.065	1.00	41.61	D
5	ATOM	7670	CA	PHE	D	522	150.263	18.902	35.500	1.00	40.23	D
	ATOM	7671	CB	PHE	D	522	151.606	18.630	36.163	1.00	40.93	D
	ATOM	7672	CG	PHE	D	522	151.580	18.761	37.646	1.00	41.77	D
	ATOM	7673	CD1	PHE	D	522	150.784	17.923	38.415	1.00	42.70	D
	ATOM	7674	CD2	PHE	D	522	152.362	19.716	38.280	1.00	42.48	D
10	ATOM	7675	CE1	PHE	D	522	150.770	18.030	39.800	1.00	43.11	D
	ATOM	7676	CE2	PHE	D	522	152.357	19.835	39.665	1.00	43.56	D
	ATOM	7677	CZ	PHE	D	522	151.559	18.989	40.427	1.00	44.10	D
	ATOM	7678	C	PHE	D	522	149.682	20.218	36.013	1.00	38.95	D
	ATOM	7679	O	PHE	D	522	149.994	21.271	35.470	1.00	38.64	D
15	ATOM	7680	N	VAL	D	523	148.823	20.169	37.028	1.00	38.34	D
	ATOM	7681	CA	VAL	D	523	148.256	21.407	37.559	1.00	38.44	D
	ATOM	7682	CB	VAL	D	523	146.720	21.500	37.351	1.00	37.33	D
	ATOM	7683	CG1	VAL	D	523	146.352	21.189	35.900	1.00	35.81	D
	ATOM	7684	CG2	VAL	D	523	146.020	20.585	38.298	1.00	39.53	D
20	ATOM	7685	C	VAL	D	523	148.543	21.590	39.044	1.00	38.09	D
	ATOM	7686	O	VAL	D	523	148.774	22.712	39.510	1.00	38.38	D
	ATOM	7687	N	GLY	D	524	148.543	20.484	39.780	1.00	36.48	D
	ATOM	7688	CA	GLY	D	524	148.798	20.567	41.203	1.00	35.67	D
	ATOM	7689	C	GLY	D	524	148.389	19.349	42.012	1.00	34.74	D
25	ATOM	7690	O	GLY	D	524	147.705	18.446	41.512	1.00	36.14	D
	ATOM	7691	N	VAL	D	525	148.812	19.351	43.276	1.00	32.26	D
	ATOM	7692	CA	VAL	D	525	148.563	18.270	44.224	1.00	28.84	D
	ATOM	7693	CB	VAL	D	525	149.834	17.940	44.980	1.00	28.68	D
	ATOM	7694	CG1	VAL	D	525	149.536	16.914	46.060	1.00	28.23	D
30	ATOM	7695	CG2	VAL	D	525	150.913	17.467	43.993	1.00	27.71	D
	ATOM	7696	C	VAL	D	525	147.522	18.613	45.261	1.00	27.86	D
	ATOM	7697	O	VAL	D	525	147.686	19.580	45.985	1.00	29.26	D
	ATOM	7698	N	LEU	D	526	146.469	17.807	45.349	1.00	26.79	D
	ATOM	7699	CA	LEU	D	526	145.421	18.028	46.341	1.00	24.97	D
35	ATOM	7700	CB	LEU	D	526	144.082	17.539	45.796	1.00	24.09	D
	ATOM	7701	CG	LEU	D	526	143.105	18.496	45.072	1.00	25.53	D
	ATOM	7702	CD1	LEU	D	526	143.706	19.861	44.714	1.00	21.96	D
	ATOM	7703	CD2	LEU	D	526	142.600	17.770	43.842	1.00	24.82	D
	ATOM	7704	C	LEU	D	526	145.771	17.305	47.659	1.00	25.98	D
40	ATOM	7705	O	LEU	D	526	145.389	16.153	47.865	1.00	26.01	D
	ATOM	7706	N	ARG	D	527	146.507	18.008	48.533	1.00	26.45	D
	ATOM	7707	CA	ARG	D	527	146.953	17.504	49.839	1.00	27.15	D
	ATOM	7708	CB	ARG	D	527	148.068	18.359	50.423	1.00	29.53	D
	ATOM	7709	CG	ARG	D	527	149.136	18.793	49.481	1.00	30.78	D
45	ATOM	7710	CD	ARG	D	527	150.199	17.750	49.353	1.00	29.79	D
	ATOM	7711	NE	ARG	D	527	151.289	18.254	48.534	1.00	28.82	D
	ATOM	7712	CZ	ARG	D	527	152.426	17.609	48.341	1.00	28.06	D
	ATOM	7713	NH1	ARG	D	527	152.621	16.424	48.913	1.00	27.74	D
	ATOM	7714	NH2	ARG	D	527	153.361	18.156	47.578	1.00	28.96	D
50	ATOM	7715	C	ARG	D	527	145.833	17.583	50.854	1.00	27.48	D
	ATOM	7716	O	ARG	D	527	145.198	18.625	50.982	1.00	28.10	D
	ATOM	7717	N	GLY	D	528	145.643	16.511	51.618	1.00	27.13	D
	ATOM	7718	CA	GLY	D	528	144.593	16.502	52.618	1.00	25.97	D
	ATOM	7719	C	GLY	D	528	144.378	15.186	53.350	1.00	27.12	D

	ATOM	7720	O	GLY	D	528	144.222	15.170	54.573	1.00	26.85	D
	ATOM	7721	N	HIS	D	529	144.349	14.076	52.619	1.00	28.35	D
	ATOM	7722	CA	HIS	D	529	144.148	12.771	53.242	1.00	28.78	D
	ATOM	7723	CB	HIS	D	529	143.686	11.747	52.197	1.00	29.36	D
5	ATOM	7724	CG	HIS	D	529	142.272	11.942	51.729	1.00	31.01	D
	ATOM	7725	CD2	HIS	D	529	141.776	12.234	50.502	1.00	32.50	D
	ATOM	7726	ND1	HIS	D	529	141.181	11.808	52.562	1.00	29.94	D
	ATOM	7727	CE1	HIS	D	529	140.074	12.010	51.864	1.00	32.77	D
	ATOM	7728	NE2	HIS	D	529	140.409	12.270	50.613	1.00	31.73	D
10	ATOM	7729	C	HIS	D	529	145.428	12.293	53.922	1.00	29.06	D
	ATOM	7730	O	HIS	D	529	146.525	12.716	53.562	1.00	29.97	D
	ATOM	7731	N	MSE	D	530	145.278	11.412	54.906	1.00	30.41	D
	ATOM	7732	CA	MSE	D	530	146.411	10.872	55.662	1.00	31.44	D
	ATOM	7733	CB	MSE	D	530	146.116	10.979	57.163	1.00	36.54	D
15	ATOM	7734	CG	MSE	D	530	145.727	12.383	57.647	1.00	40.77	D
	ATOM	7735	SE	MSE	D	530	147.225	13.555	57.992	1.00	48.72	D
	ATOM	7736	CE	MSE	D	530	147.747	12.886	59.726	1.00	44.45	D
	ATOM	7737	C	MSE	D	530	146.708	9.409	55.286	1.00	30.15	D
	ATOM	7738	O	MSE	D	530	147.663	8.804	55.770	1.00	31.06	D
20	ATOM	7739	N	ALA	D	531	145.872	8.837	54.433	1.00	27.91	D
	ATOM	7740	CA	ALA	D	531	146.077	7.470	53.983	1.00	25.52	D
	ATOM	7741	CB	ALA	D	531	145.322	6.506	54.863	1.00	23.17	D
	ATOM	7742	C	ALA	D	531	145.634	7.329	52.528	1.00	25.05	D
	ATOM	7743	O	ALA	D	531	145.166	8.283	51.903	1.00	25.19	D
25	ATOM	7744	N	SER	D	532	145.778	6.126	52.004	1.00	24.01	D
	ATOM	7745	CA	SER	D	532	145.431	5.834	50.635	1.00	23.62	D
	ATOM	7746	CB	SER	D	532	145.452	4.332	50.427	1.00	23.66	D
	ATOM	7747	OG	SER	D	532	145.044	4.009	49.120	1.00	24.72	D
	ATOM	7748	C	SER	D	532	144.093	6.391	50.161	1.00	24.24	D
30	ATOM	7749	O	SER	D	532	143.059	6.249	50.835	1.00	23.67	D
	ATOM	7750	N	VAL	D	533	144.131	7.028	48.987	1.00	22.26	D
	ATOM	7751	CA	VAL	D	533	142.930	7.588	48.383	1.00	21.80	D
	ATOM	7752	CB	VAL	D	533	143.238	8.790	47.509	1.00	19.37	D
	ATOM	7753	CG1	VAL	D	533	141.973	9.225	46.786	1.00	19.14	D
35	ATOM	7754	CG2	VAL	D	533	143.757	9.912	48.367	1.00	16.33	D
	ATOM	7755	C	VAL	D	533	142.311	6.476	47.564	1.00	23.09	D
	ATOM	7756	O	VAL	D	533	142.740	6.181	46.464	1.00	24.67	D
	ATOM	7757	N	ARG	D	534	141.281	5.865	48.125	1.00	23.37	D
	ATOM	7758	CA	ARG	D	534	140.630	4.734	47.514	1.00	21.94	D
40	ATOM	7759	CB	ARG	D	534	139.887	3.966	48.588	1.00	22.94	D
	ATOM	7760	CG	ARG	D	534	139.334	2.660	48.104	1.00	20.89	D
	ATOM	7761	CD	ARG	D	534	140.460	1.735	47.688	1.00	20.13	D
	ATOM	7762	NE	ARG	D	534	139.934	0.404	47.470	1.00	22.05	D
	ATOM	7763	CZ	ARG	D	534	139.177	0.061	46.435	1.00	21.88	D
45	ATOM	7764	NH1	ARG	D	534	138.859	0.955	45.499	1.00	16.38	D
	ATOM	7765	NH2	ARG	D	534	138.723	-1.184	46.354	1.00	21.24	D
	ATOM	7766	C	ARG	D	534	139.687	4.934	46.350	1.00	21.77	D
	ATOM	7767	O	ARG	D	534	139.630	4.082	45.464	1.00	23.87	D
	ATOM	7768	N	THR	D	535	138.944	6.029	46.328	1.00	21.46	D
50	ATOM	7769	CA	THR	D	535	137.976	6.186	45.252	1.00	23.21	D
	ATOM	7770	CB	THR	D	535	136.630	5.607	45.693	1.00	22.72	D
	ATOM	7771	OG1	THR	D	535	135.615	5.908	44.728	1.00	24.25	D
	ATOM	7772	CG2	THR	D	535	136.255	6.189	47.038	1.00	21.59	D
	ATOM	7773	C	THR	D	535	137.785	7.623	44.871	1.00	22.36	D

	ATOM	7774	O	THR	D	535	138.010	8.494	45.692	1.00	22.27	D
	ATOM	7775	N	VAL	D	536	137.383	7.869	43.627	1.00	23.47	D
	ATOM	7776	CA	VAL	D	536	137.154	9.240	43.178	1.00	26.56	D
	ATOM	7777	CB	VAL	D	536	138.340	9.805	42.381	1.00	27.30	D
5	ATOM	7778	CG1	VAL	D	536	138.152	11.303	42.178	1.00	27.76	D
	ATOM	7779	CG2	VAL	D	536	139.615	9.573	43.126	1.00	29.04	D
	ATOM	7780	C	VAL	D	536	135.907	9.379	42.330	1.00	26.74	D
	ATOM	7781	O	VAL	D	536	135.550	8.486	41.558	1.00	28.31	D
	ATOM	7782	N	SER	D	537	135.248	10.517	42.473	1.00	26.29	D
10	ATOM	7783	CA	SER	D	537	134.019	10.759	41.741	1.00	25.58	D
	ATOM	7784	CB	SER	D	537	132.832	10.197	42.529	1.00	23.69	D
	ATOM	7785	OG	SER	D	537	131.605	10.436	41.878	1.00	19.22	D
	ATOM	7786	C	SER	D	537	133.859	12.252	41.547	1.00	26.69	D
	ATOM	7787	O	SER	D	537	133.697	13.000	42.517	1.00	27.22	D
15	ATOM	7788	N	GLY	D	538	133.923	12.684	40.294	1.00	26.82	D
	ATOM	7789	CA	GLY	D	538	133.794	14.096	40.020	1.00	28.64	D
	ATOM	7790	C	GLY	D	538	133.027	14.446	38.766	1.00	28.83	D
	ATOM	7791	O	GLY	D	538	132.961	13.666	37.820	1.00	29.17	D
	ATOM	7792	N	HIS	D	539	132.450	15.645	38.790	1.00	29.15	D
20	ATOM	7793	CA	HIS	D	539	131.679	16.226	37.696	1.00	27.88	D
	ATOM	7794	CB	HIS	D	539	130.179	16.025	37.911	1.00	27.43	D
	ATOM	7795	CG	HIS	D	539	129.333	16.567	36.799	1.00	28.11	D
	ATOM	7796	CD2	HIS	D	539	128.736	17.772	36.637	1.00	30.46	D
	ATOM	7797	ND1	HIS	D	539	129.046	15.843	35.662	1.00	27.67	D
25	ATOM	7798	CE1	HIS	D	539	128.307	16.577	34.848	1.00	29.05	D
	ATOM	7799	NE2	HIS	D	539	128.105	17.753	35.415	1.00	30.92	D
	ATOM	7800	C	HIS	D	539	131.959	17.735	37.697	1.00	29.12	D
	ATOM	7801	O	HIS	D	539	131.791	18.409	38.728	1.00	28.57	D
	ATOM	7802	N	GLY	D	540	132.376	18.261	36.546	1.00	28.54	D
30	ATOM	7803	CA	GLY	D	540	132.650	19.682	36.436	1.00	27.08	D
	ATOM	7804	C	GLY	D	540	133.872	20.122	37.215	1.00	27.09	D
	ATOM	7805	O	GLY	D	540	134.904	19.454	37.179	1.00	28.54	D
	ATOM	7806	N	ASN	D	541	133.777	21.245	37.920	1.00	25.16	D
	ATOM	7807	CA	ASN	D	541	134.924	21.706	38.679	1.00	24.86	D
35	ATOM	7808	CB	ASN	D	541	134.907	23.237	38.816	1.00	26.35	D
	ATOM	7809	CG	ASN	D	541	133.889	23.726	39.851	1.00	29.47	D
	ATOM	7810	OD1	ASN	D	541	132.706	23.341	39.803	1.00	29.21	D
	ATOM	7811	ND2	ASN	D	541	134.341	24.575	40.792	1.00	26.35	D
	ATOM	7812	C	ASN	D	541	134.915	21.062	40.056	1.00	24.63	D
40	ATOM	7813	O	ASN	D	541	135.803	21.308	40.864	1.00	25.54	D
	ATOM	7814	N	ILE	D	542	133.921	20.220	40.321	1.00	22.93	D
	ATOM	7815	CA	ILE	D	542	133.821	19.574	41.629	1.00	22.46	D
	ATOM	7816	CB	ILE	D	542	132.361	19.724	42.186	1.00	20.91	D
	ATOM	7817	CG2	ILE	D	542	132.215	18.977	43.497	1.00	22.05	D
45	ATOM	7818	CG1	ILE	D	542	132.001	21.215	42.385	1.00	19.70	D
	ATOM	7819	CD1	ILE	D	542	132.866	22.016	43.388	1.00	10.85	D
	ATOM	7820	C	ILE	D	542	134.258	18.085	41.663	1.00	24.27	D
	ATOM	7821	O	ILE	D	542	133.841	17.258	40.832	1.00	23.68	D
	ATOM	7822	N	VAL	D	543	135.108	17.738	42.624	1.00	24.95	D
50	ATOM	7823	CA	VAL	D	543	135.565	16.350	42.735	1.00	26.33	D
	ATOM	7824	CB	VAL	D	543	137.023	16.176	42.199	1.00	28.00	D
	ATOM	7825	CG1	VAL	D	543	137.492	14.742	42.406	1.00	27.16	D
	ATOM	7826	CG2	VAL	D	543	137.073	16.515	40.716	1.00	30.18	D
	ATOM	7827	C	VAL	D	543	135.509	15.864	44.174	1.00	25.02	D

	ATOM	7828	O	VAL	D	543	135.893	16.601	45.079	1.00	24.45	D
	ATOM	7829	N	VAL	D	544	135.017	14.639	44.388	1.00	24.93	D
	ATOM	7830	CA	VAL	D	544	134.939	14.093	45.748	1.00	25.31	D
	ATOM	7831	CB	VAL	D	544	133.495	13.783	46.197	1.00	24.60	D
5	ATOM	7832	CG1	VAL	D	544	133.507	13.509	47.679	1.00	24.71	D
	ATOM	7833	CG2	VAL	D	544	132.553	14.940	45.889	1.00	25.25	D
	ATOM	7834	C	VAL	D	544	135.750	12.814	45.910	1.00	25.25	D
	ATOM	7835	O	VAL	D	544	135.662	11.903	45.082	1.00	26.67	D
	ATOM	7836	N	SER	D	545	136.534	12.745	46.985	1.00	24.15	D
10	ATOM	7837	CA	SER	D	545	137.367	11.566	47.236	1.00	24.66	D
	ATOM	7838	CB	SER	D	545	138.835	11.960	47.213	1.00	22.85	D
	ATOM	7839	OG	SER	D	545	139.110	12.914	48.221	1.00	26.17	D
	ATOM	7840	C	SER	D	545	137.105	10.777	48.525	1.00	26.03	D
	ATOM	7841	O	SER	D	545	136.609	11.315	49.516	1.00	27.76	D
15	ATOM	7842	N	GLY	D	546	137.467	9.497	48.495	1.00	25.26	D
	ATOM	7843	CA	GLY	D	546	137.292	8.642	49.647	1.00	24.44	D
	ATOM	7844	C	GLY	D	546	138.637	8.073	50.039	1.00	24.54	D
	ATOM	7845	O	GLY	D	546	139.318	7.450	49.220	1.00	23.24	D
	ATOM	7846	N	SER	D	547	139.038	8.282	51.288	1.00	25.20	D
20	ATOM	7847	CA	SER	D	547	140.339	7.773	51.730	1.00	27.40	D
	ATOM	7848	CB	SER	D	547	141.235	8.897	52.239	1.00	25.06	D
	ATOM	7849	OG	SER	D	547	142.424	8.333	52.763	1.00	23.13	D
	ATOM	7850	C	SER	D	547	140.286	6.723	52.816	1.00	28.75	D
	ATOM	7851	O	SER	D	547	139.260	6.520	53.462	1.00	32.39	D
25	ATOM	7852	N	TYR	D	548	141.411	6.062	53.031	1.00	27.35	D
	ATOM	7853	CA	TYR	D	548	141.457	5.071	54.078	1.00	24.34	D
	ATOM	7854	CB	TYR	D	548	142.588	4.085	53.835	1.00	21.23	D
	ATOM	7855	CG	TYR	D	548	142.185	2.933	52.964	1.00	18.24	D
	ATOM	7856	CD1	TYR	D	548	140.975	2.940	52.267	1.00	17.37	D
30	ATOM	7857	CE1	TYR	D	548	140.631	1.894	51.426	1.00	15.22	D
	ATOM	7858	CD2	TYR	D	548	143.030	1.850	52.802	1.00	18.07	D
	ATOM	7859	CE2	TYR	D	548	142.701	0.796	51.969	1.00	15.33	D
	ATOM	7860	CZ	TYR	D	548	141.507	0.825	51.283	1.00	17.35	D
	ATOM	7861	OH	TYR	D	548	141.195	-0.213	50.435	1.00	18.41	D
35	ATOM	7862	C	TYR	D	548	141.637	5.742	55.428	1.00	25.52	D
	ATOM	7863	O	TYR	D	548	141.897	5.060	56.401	1.00	24.80	D
	ATOM	7864	N	ASP	D	549	141.517	7.070	55.496	1.00	26.28	D
	ATOM	7865	CA	ASP	D	549	141.637	7.739	56.789	1.00	26.66	D
	ATOM	7866	CB	ASP	D	549	142.332	9.114	56.693	1.00	28.11	D
40	ATOM	7867	CG	ASP	D	549	141.761	10.006	55.611	1.00	28.18	D
	ATOM	7868	OD1	ASP	D	549	140.580	9.822	55.227	1.00	30.65	D
	ATOM	7869	OD2	ASP	D	549	142.507	10.909	55.167	1.00	25.41	D
	ATOM	7870	C	ASP	D	549	140.239	7.884	57.363	1.00	26.46	D
	ATOM	7871	O	ASP	D	549	140.014	8.634	58.311	1.00	26.79	D
45	ATOM	7872	N	ASN	D	550	139.309	7.157	56.742	1.00	26.14	D
	ATOM	7873	CA	ASN	D	550	137.906	7.115	57.139	1.00	24.53	D
	ATOM	7874	CB	ASN	D	550	137.825	6.849	58.633	1.00	23.45	D
	ATOM	7875	CG	ASN	D	550	138.484	5.542	59.012	1.00	23.88	D
	ATOM	7876	OD1	ASN	D	550	139.126	4.894	58.190	1.00	24.66	D
50	ATOM	7877	ND2	ASN	D	550	138.319	5.143	60.253	1.00	25.10	D
	ATOM	7878	C	ASN	D	550	137.162	8.374	56.796	1.00	23.51	D
	ATOM	7879	O	ASN	D	550	136.006	8.534	57.146	1.00	23.99	D
	ATOM	7880	N	THR	D	551	137.811	9.237	56.038	1.00	24.61	D
	ATOM	7881	CA	THR	D	551	137.221	10.510	55.706	1.00	24.98	D

	ATOM	7882	CB	THR	D	551	138.155	11.584	56.208	1.00	25.84	D
	ATOM	7883	OG1	THR	D	551	137.402	12.640	56.803	1.00	26.76	D
	ATOM	7884	CG2	THR	D	551	139.015	12.107	55.053	1.00	24.97	D
	ATOM	7885	C	THR	D	551	136.993	10.725	54.206	1.00	25.92	D
5	ATOM	7886	O	THR	D	551	137.535	9.996	53.376	1.00	24.99	D
	ATOM	7887	N	LEU	D	552	136.173	11.719	53.868	1.00	26.68	D
	ATOM	7888	CA	LEU	D	552	135.934	12.079	52.471	1.00	26.79	D
	ATOM	7889	CB	LEU	D	552	134.508	11.771	52.031	1.00	24.86	D
	ATOM	7890	CG	LEU	D	552	134.189	10.328	51.665	1.00	23.77	D
10	ATOM	7891	CD1	LEU	D	552	133.215	9.804	52.689	1.00	23.78	D
	ATOM	7892	CD2	LEU	D	552	133.597	10.237	50.257	1.00	22.54	D
	ATOM	7893	C	LEU	D	552	136.180	13.572	52.308	1.00	27.51	D
	ATOM	7894	O	LEU	D	552	135.792	14.366	53.170	1.00	28.40	D
	ATOM	7895	N	ILE	D	553	136.828	13.955	51.206	1.00	27.13	D
15	ATOM	7896	CA	ILE	D	553	137.102	15.372	50.939	1.00	25.65	D
	ATOM	7897	CB	ILE	D	553	138.623	15.686	50.957	1.00	24.82	D
	ATOM	7898	CG2	ILE	D	553	138.854	17.153	50.606	1.00	24.33	D
	ATOM	7899	CG1	ILE	D	553	139.212	15.444	52.355	1.00	25.26	D
	ATOM	7900	CD1	ILE	D	553	140.725	15.613	52.413	1.00	24.18	D
20	ATOM	7901	C	ILE	D	553	136.531	15.869	49.606	1.00	25.82	D
	ATOM	7902	O	ILE	D	553	136.664	15.210	48.561	1.00	24.35	D
	ATOM	7903	N	VAL	D	554	135.889	17.038	49.672	1.00	24.96	D
	ATOM	7904	CA	VAL	D	554	135.299	17.704	48.503	1.00	24.79	D
	ATOM	7905	CB	VAL	D	554	133.964	18.425	48.858	1.00	21.69	D
25	ATOM	7906	CG1	VAL	D	554	133.366	19.041	47.620	1.00	19.43	D
	ATOM	7907	CG2	VAL	D	554	133.000	17.455	49.480	1.00	21.35	D
	ATOM	7908	C	VAL	D	554	136.308	18.753	48.016	1.00	26.46	D
	ATOM	7909	O	VAL	D	554	136.646	19.689	48.746	1.00	26.64	D
	ATOM	7910	N	TRP	D	555	136.812	18.574	46.797	1.00	27.69	D
30	ATOM	7911	CA	TRP	D	555	137.784	19.500	46.233	1.00	28.09	D
	ATOM	7912	CB	TRP	D	555	139.026	18.767	45.703	1.00	28.18	D
	ATOM	7913	CG	TRP	D	555	139.593	17.681	46.576	1.00	29.63	D
	ATOM	7914	CD2	TRP	D	555	140.695	17.795	47.487	1.00	30.60	D
	ATOM	7915	CE2	TRP	D	555	140.948	16.505	48.003	1.00	30.79	D
35	ATOM	7916	CE3	TRP	D	555	141.492	18.862	47.915	1.00	30.24	D
	ATOM	7917	CD1	TRP	D	555	139.228	16.365	46.587	1.00	29.55	D
	ATOM	7918	NE1	TRP	D	555	140.041	15.652	47.436	1.00	30.90	D
	ATOM	7919	CZ2	TRP	D	555	141.968	16.253	48.921	1.00	31.50	D
	ATOM	7920	CZ3	TRP	D	555	142.510	18.608	48.832	1.00	31.00	D
40	ATOM	7921	CH2	TRP	D	555	142.736	17.314	49.323	1.00	31.35	D
	ATOM	7922	C	TRP	D	555	137.210	20.306	45.075	1.00	27.75	D
	ATOM	7923	O	TRP	D	555	136.392	19.807	44.297	1.00	26.08	D
	ATOM	7924	N	ASP	D	556	137.658	21.556	44.981	1.00	29.07	D
	ATOM	7925	CA	ASP	D	556	137.274	22.463	43.904	1.00	29.82	D
45	ATOM	7926	CB	ASP	D	556	136.917	23.849	44.425	1.00	33.43	D
	ATOM	7927	CG	ASP	D	556	136.336	24.762	43.335	1.00	36.51	D
	ATOM	7928	OD1	ASP	D	556	136.913	24.864	42.216	1.00	35.80	D
	ATOM	7929	OD2	ASP	D	556	135.285	25.388	43.609	1.00	39.49	D
	ATOM	7930	C	ASP	D	556	138.539	22.591	43.095	1.00	28.83	D
50	ATOM	7931	O	ASP	D	556	139.440	23.337	43.463	1.00	25.39	D
	ATOM	7932	N	VAL	D	557	138.596	21.858	41.995	1.00	31.59	D
	ATOM	7933	CA	VAL	D	557	139.756	21.853	41.123	1.00	34.16	D
	ATOM	7934	CB	VAL	D	557	139.592	20.840	40.007	1.00	34.22	D
	ATOM	7935	CG1	VAL	D	557	140.777	20.942	39.064	1.00	36.74	D

	ATOM	7936	CG2	VAL	D	557	139.460	19.444	40.582	1.00	31.24	D
	ATOM	7937	C	VAL	D	557	140.021	23.183	40.466	1.00	35.74	D
	ATOM	7938	O	VAL	D	557	141.168	23.535	40.244	1.00	37.94	D
	ATOM	7939	N	ALA	D	558	138.959	23.906	40.133	1.00	37.02	D
5	ATOM	7940	CA	ALA	D	558	139.107	25.196	39.485	1.00	37.13	D
	ATOM	7941	CB	ALA	D	558	137.747	25.730	39.065	1.00	39.25	D
	ATOM	7942	C	ALA	D	558	139.784	26.167	40.430	1.00	36.58	D
	ATOM	7943	O	ALA	D	558	140.342	27.168	39.997	1.00	37.02	D
	ATOM	7944	N	GLN	D	559	139.729	25.857	41.722	1.00	37.85	D
10	ATOM	7945	CA	GLN	D	559	140.327	26.688	42.763	1.00	37.56	D
	ATOM	7946	CB	GLN	D	559	139.248	27.110	43.750	1.00	37.90	D
	ATOM	7947	CG	GLN	D	559	139.672	28.264	44.624	1.00	43.44	D
	ATOM	7948	CD	GLN	D	559	138.523	28.874	45.444	1.00	45.28	D
	ATOM	7949	OE1	GLN	D	559	137.375	28.927	44.987	1.00	46.49	D
15	ATOM	7950	NE2	GLN	D	559	138.839	29.354	46.655	1.00	45.82	D
	ATOM	7951	C	GLN	D	559	141.419	25.896	43.479	1.00	37.70	D
	ATOM	7952	O	GLN	D	559	142.131	26.428	44.336	1.00	36.85	D
	ATOM	7953	N	MSE	D	560	141.535	24.624	43.094	1.00	38.22	D
	ATOM	7954	CA	MSE	D	560	142.505	23.687	43.645	1.00	37.94	D
20	ATOM	7955	CB	MSE	D	560	143.870	23.912	42.984	1.00	37.36	D
	ATOM	7956	CG	MSE	D	560	144.681	22.648	42.719	1.00	37.70	D
	ATOM	7957	SE	MSE	D	560	143.786	21.540	41.377	1.00	39.17	D
	ATOM	7958	CE	MSE	D	560	143.835	22.738	39.886	1.00	41.26	D
	ATOM	7959	C	MSE	D	560	142.597	23.865	45.164	1.00	37.81	D
25	ATOM	7960	O	MSE	D	560	143.675	24.035	45.710	1.00	39.53	D
	ATOM	7961	N	LYS	D	561	141.449	23.844	45.832	1.00	37.74	D
	ATOM	7962	CA	LYS	D	561	141.384	23.995	47.279	1.00	38.73	D
	ATOM	7963	CB	LYS	D	561	141.037	25.452	47.638	1.00	39.81	D
	ATOM	7964	CG	LYS	D	561	142.191	26.428	47.399	0.00	40.07	D
30	ATOM	7965	CD	LYS	D	561	143.372	26.124	48.318	0.00	40.65	D
	ATOM	7966	CE	LYS	D	561	142.998	26.355	49.774	0.00	41.01	D
	ATOM	7967	NZ	LYS	D	561	144.024	25.827	50.715	0.00	41.29	D
	ATOM	7968	C	LYS	D	561	140.356	23.022	47.887	1.00	39.22	D
	ATOM	7969	O	LYS	D	561	139.419	22.584	47.208	1.00	38.84	D
35	ATOM	7970	N	CYS	D	562	140.556	22.670	49.159	1.00	38.90	D
	ATOM	7971	CA	CYS	D	562	139.668	21.759	49.885	1.00	38.52	D
	ATOM	7972	CB	CYS	D	562	140.360	21.270	51.164	1.00	38.67	D
	ATOM	7973	SG	CYS	D	562	139.309	20.275	52.277	1.00	44.51	D
	ATOM	7974	C	CYS	D	562	138.402	22.521	50.260	1.00	37.58	D
40	ATOM	7975	O	CYS	D	562	138.494	23.572	50.888	1.00	40.09	D
	ATOM	7976	N	LEU	D	563	137.223	22.015	49.895	1.00	34.69	D
	ATOM	7977	CA	LEU	D	563	135.981	22.726	50.232	1.00	31.60	D
	ATOM	7978	CB	LEU	D	563	134.924	22.550	49.132	1.00	28.39	D
	ATOM	7979	CG	LEU	D	563	135.214	23.279	47.820	1.00	25.92	D
45	ATOM	7980	CD1	LEU	D	563	133.986	23.317	46.939	1.00	24.65	D
	ATOM	7981	CD2	LEU	D	563	135.679	24.670	48.139	1.00	23.99	D
	ATOM	7982	C	LEU	D	563	135.388	22.281	51.552	1.00	30.82	D
	ATOM	7983	O	LEU	D	563	135.012	23.099	52.388	1.00	29.72	D
	ATOM	7984	N	TYR	D	564	135.320	20.968	51.723	1.00	31.20	D
50	ATOM	7985	CA	TYR	D	564	134.768	20.358	52.915	1.00	29.79	D
	ATOM	7986	CB	TYR	D	564	133.276	20.087	52.705	1.00	31.53	D
	ATOM	7987	CG	TYR	D	564	132.415	21.316	52.480	1.00	35.18	D
	ATOM	7988	CD1	TYR	D	564	132.216	22.250	53.503	1.00	35.47	D
	ATOM	7989	CE1	TYR	D	564	131.381	23.356	53.321	1.00	37.11	D

	ATOM	7990	CD2	TYR	D	564	131.757	21.522	51.257	1.00	35.79	D
	ATOM	7991	CE2	TYR	D	564	130.918	22.626	51.064	1.00	37.32	D
	ATOM	7992	CZ	TYR	D	564	130.733	23.539	52.100	1.00	37.56	D
	ATOM	7993	OH	TYR	D	564	129.901	24.625	51.926	1.00	37.99	D
5	ATOM	7994	C	TYR	D	564	135.464	19.028	53.213	1.00	28.42	D
	ATOM	7995	O	TYR	D	564	135.998	18.357	52.323	1.00	29.93	D
	ATOM	7996	N	ILE	D	565	135.448	18.655	54.482	1.00	26.22	D
	ATOM	7997	CA	ILE	D	565	136.001	17.389	54.916	1.00	24.23	D
	ATOM	7998	CB	ILE	D	565	137.222	17.574	55.861	1.00	24.90	D
10	ATOM	7999	CG2	ILE	D	565	137.641	16.232	56.471	1.00	22.64	D
	ATOM	8000	CG1	ILE	D	565	138.389	18.173	55.066	1.00	23.83	D
	ATOM	8001	CD1	ILE	D	565	139.596	18.476	55.898	1.00	22.10	D
	ATOM	8002	C	ILE	D	565	134.853	16.708	55.654	1.00	24.14	D
	ATOM	8003	O	ILE	D	565	134.436	17.123	56.745	1.00	24.92	D
15	ATOM	8004	N	LEU	D	566	134.319	15.674	55.022	1.00	23.68	D
	ATOM	8005	CA	LEU	D	566	133.209	14.910	55.567	1.00	21.44	D
	ATOM	8006	CB	LEU	D	566	132.498	14.204	54.433	1.00	18.60	D
	ATOM	8007	CG	LEU	D	566	132.249	15.108	53.240	1.00	16.04	D
	ATOM	8008	CD1	LEU	D	566	131.493	14.312	52.195	1.00	18.64	D
20	ATOM	8009	CD2	LEU	D	566	131.471	16.327	53.661	1.00	11.95	D
	ATOM	8010	C	LEU	D	566	133.725	13.876	56.532	1.00	20.93	D
	ATOM	8011	O	LEU	D	566	134.448	12.975	56.126	1.00	21.77	D
	ATOM	8012	N	SER	D	567	133.345	13.980	57.800	1.00	22.31	D
	ATOM	8013	CA	SER	D	567	133.806	12.995	58.783	1.00	23.94	D
25	ATOM	8014	CB	SER	D	567	134.810	13.630	59.731	1.00	23.34	D
	ATOM	8015	OG	SER	D	567	135.808	14.311	58.987	1.00	24.18	D
	ATOM	8016	C	SER	D	567	132.676	12.349	59.568	1.00	24.28	D
	ATOM	8017	O	SER	D	567	131.586	12.904	59.663	1.00	24.81	D
	ATOM	8018	N	GLY	D	568	132.950	11.166	60.113	1.00	25.74	D
30	ATOM	8019	CA	GLY	D	568	131.953	10.416	60.858	1.00	25.21	D
	ATOM	8020	C	GLY	D	568	132.134	8.906	60.681	1.00	26.37	D
	ATOM	8021	O	GLY	D	568	132.130	8.163	61.664	1.00	27.73	D
	ATOM	8022	N	HIS	D	569	132.288	8.440	59.437	1.00	25.07	D
	ATOM	8023	CA	HIS	D	569	132.500	7.007	59.175	1.00	23.33	D
35	ATOM	8024	CB	HIS	D	569	132.949	6.749	57.730	1.00	22.22	D
	ATOM	8025	CG	HIS	D	569	131.839	6.801	56.725	1.00	21.96	D
	ATOM	8026	CD2	HIS	D	569	131.594	7.675	55.720	1.00	21.82	D
	ATOM	8027	ND1	HIS	D	569	130.827	5.865	56.671	1.00	20.28	D
	ATOM	8028	CE1	HIS	D	569	130.009	6.160	55.676	1.00	20.59	D
40	ATOM	8029	NE2	HIS	D	569	130.452	7.254	55.083	1.00	20.12	D
	ATOM	8030	C	HIS	D	569	133.590	6.520	60.129	1.00	24.25	D
	ATOM	8031	O	HIS	D	569	134.625	7.176	60.291	1.00	24.38	D
	ATOM	8032	N	THR	D	570	133.357	5.371	60.759	1.00	25.24	D
	ATOM	8033	CA	THR	D	570	134.296	4.806	61.724	1.00	25.54	D
45	ATOM	8034	CB	THR	D	570	133.508	4.097	62.867	1.00	26.19	D
	ATOM	8035	OG1	THR	D	570	132.385	3.381	62.321	1.00	27.58	D
	ATOM	8036	CG2	THR	D	570	133.008	5.120	63.869	1.00	23.79	D
	ATOM	8037	C	THR	D	570	135.355	3.864	61.114	1.00	25.50	D
	ATOM	8038	O	THR	D	570	136.225	3.349	61.812	1.00	26.67	D
50	ATOM	8039	N	ASP	D	571	135.279	3.628	59.811	1.00	26.22	D
	ATOM	8040	CA	ASP	D	571	136.284	2.804	59.141	1.00	25.18	D
	ATOM	8041	CB	ASP	D	571	135.810	1.365	58.999	1.00	26.72	D
	ATOM	8042	CG	ASP	D	571	136.956	0.386	59.009	1.00	28.41	D
	ATOM	8043	OD1	ASP	D	571	138.011	0.726	58.447	1.00	30.11	D

	ATOM	8044	OD2	ASP	D	571	136.818	-0.715	59.575	1.00	29.31	D
	ATOM	8045	C	ASP	D	571	136.590	3.382	57.759	1.00	24.07	D
	ATOM	8046	O	ASP	D	571	135.917	4.303	57.281	1.00	22.39	D
	ATOM	8047	N	ARG	D	572	137.593	2.825	57.101	1.00	23.27	D
5	ATOM	8048	CA	ARG	D	572	137.976	3.314	55.781	1.00	22.84	D
	ATOM	8049	CB	ARG	D	572	139.153	2.491	55.250	1.00	21.15	D
	ATOM	8050	CG	ARG	D	572	138.981	1.032	55.408	1.00	19.04	D
	ATOM	8051	CD	ARG	D	572	140.058	0.268	54.705	1.00	20.64	D
	ATOM	8052	NE	ARG	D	572	141.341	0.249	55.393	1.00	22.31	D
10	ATOM	8053	CZ	ARG	D	572	142.293	-0.649	55.130	1.00	23.14	D
	ATOM	8054	NH1	ARG	D	572	142.071	-1.571	54.198	1.00	17.78	D
	ATOM	8055	NH2	ARG	D	572	143.449	-0.646	55.799	1.00	23.35	D
	ATOM	8056	C	ARG	D	572	136.820	3.300	54.789	1.00	22.51	D
	ATOM	8057	O	ARG	D	572	135.914	2.475	54.922	1.00	22.42	D
15	ATOM	8058	N	ILE	D	573	136.825	4.241	53.837	1.00	23.14	D
	ATOM	8059	CA	ILE	D	573	135.779	4.301	52.809	1.00	24.51	D
	ATOM	8060	CB	ILE	D	573	135.449	5.739	52.295	1.00	27.12	D
	ATOM	8061	CG2	ILE	D	573	134.618	5.643	51.025	0.00	26.23	D
	ATOM	8062	CG1	ILE	D	573	134.652	6.536	53.333	1.00	26.27	D
20	ATOM	8063	CD1	ILE	D	573	135.472	7.060	54.419	1.00	25.64	D
	ATOM	8064	C	ILE	D	573	136.330	3.577	51.601	1.00	24.11	D
	ATOM	8065	O	ILE	D	573	137.517	3.724	51.270	1.00	23.80	D
	ATOM	8066	N	TYR	D	574	135.459	2.830	50.927	1.00	22.78	D
	ATOM	8067	CA	TYR	D	574	135.849	2.071	49.742	1.00	22.23	D
25	ATOM	8068	CB	TYR	D	574	135.498	0.583	49.951	1.00	21.98	D
	ATOM	8069	CG	TYR	D	574	136.588	-0.242	50.619	1.00	24.35	D
	ATOM	8070	CD1	TYR	D	574	137.503	-0.992	49.853	1.00	22.37	D
	ATOM	8071	CE1	TYR	D	574	138.524	-1.729	50.463	1.00	23.23	D
	ATOM	8072	CD2	TYR	D	574	136.723	-0.254	52.019	1.00	24.83	D
30	ATOM	8073	CE2	TYR	D	574	137.736	-0.982	52.641	1.00	26.35	D
	ATOM	8074	CZ	TYR	D	574	138.639	-1.719	51.862	1.00	25.64	D
	ATOM	8075	OH	TYR	D	574	139.650	-2.423	52.493	1.00	26.87	D
	ATOM	8076	C	TYR	D	574	135.245	2.570	48.402	1.00	21.18	D
	ATOM	8077	O	TYR	D	574	135.716	2.188	47.325	1.00	22.28	D
35	ATOM	8078	N	SER	D	575	134.231	3.432	48.464	1.00	19.10	D
	ATOM	8079	CA	SER	D	575	133.556	3.933	47.258	1.00	18.07	D
	ATOM	8080	CB	SER	D	575	132.559	2.872	46.756	1.00	18.09	D
	ATOM	8081	OG	SER	D	575	131.552	3.435	45.926	1.00	17.37	D
	ATOM	8082	C	SER	D	575	132.814	5.255	47.504	1.00	17.95	D
40	ATOM	8083	O	SER	D	575	132.312	5.515	48.599	1.00	17.19	D
	ATOM	8084	N	THR	D	576	132.731	6.105	46.498	1.00	17.64	D
	ATOM	8085	CA	THR	D	576	132.009	7.334	46.737	1.00	19.01	D
	ATOM	8086	CB	THR	D	576	132.936	8.441	47.285	1.00	17.27	D
	ATOM	8087	OG1	THR	D	576	132.145	9.575	47.662	1.00	15.53	D
45	ATOM	8088	CG2	THR	D	576	133.968	8.869	46.228	1.00	20.28	D
	ATOM	8089	C	THR	D	576	131.369	7.808	45.454	1.00	19.84	D
	ATOM	8090	O	THR	D	576	131.878	7.565	44.358	1.00	20.54	D
	ATOM	8091	N	ILE	D	577	130.228	8.461	45.571	1.00	18.92	D
	ATOM	8092	CA	ILE	D	577	129.622	8.959	44.366	1.00	20.24	D
50	ATOM	8093	CB	ILE	D	577	128.395	8.161	43.984	1.00	19.47	D
	ATOM	8094	CG2	ILE	D	577	127.588	8.938	42.958	1.00	17.51	D
	ATOM	8095	CG1	ILE	D	577	128.818	6.790	43.456	1.00	19.93	D
	ATOM	8096	CD1	ILE	D	577	127.641	5.922	43.008	1.00	20.62	D
	ATOM	8097	C	ILE	D	577	129.232	10.403	44.528	1.00	21.53	D

	ATOM	8098	O	ILE	D	577	128.603	10.777	45.530	1.00	23.56	D
	ATOM	8099	N	TYR	D	578	129.615	11.223	43.551	1.00	20.82	D
	ATOM	8100	CA	TYR	D	578	129.264	12.644	43.593	1.00	21.04	D
	ATOM	8101	CB	TYR	D	578	130.384	13.509	42.982	1.00	21.65	D
5	ATOM	8102	CG	TYR	D	578	130.022	14.975	42.792	1.00	22.52	D
	ATOM	8103	CD1	TYR	D	578	129.168	15.625	43.690	1.00	22.16	D
	ATOM	8104	CE1	TYR	D	578	128.795	16.960	43.506	1.00	21.60	D
	ATOM	8105	CD2	TYR	D	578	130.510	15.702	41.701	1.00	21.12	D
	ATOM	8106	CE2	TYR	D	578	130.147	17.038	41.506	1.00	21.36	D
10	ATOM	8107	CZ	TYR	D	578	129.286	17.663	42.410	1.00	21.53	D
	ATOM	8108	OH	TYR	D	578	128.900	18.977	42.212	1.00	21.71	D
	ATOM	8109	C	TYR	D	578	127.955	12.883	42.851	1.00	20.91	D
	ATOM	8110	O	TYR	D	578	127.939	12.885	41.633	1.00	21.83	D
	ATOM	8111	N	ASP	D	579	126.866	13.094	43.596	1.00	22.68	D
15	ATOM	8112	CA	ASP	D	579	125.534	13.342	43.017	1.00	24.76	D
	ATOM	8113	CB	ASP	D	579	124.440	13.037	44.054	1.00	25.04	D
	ATOM	8114	CG	ASP	D	579	123.029	12.930	43.443	1.00	27.17	D
	ATOM	8115	OD1	ASP	D	579	122.790	13.506	42.363	1.00	26.43	D
	ATOM	8116	OD2	ASP	D	579	122.144	12.271	44.061	1.00	27.38	D
20	ATOM	8117	C	ASP	D	579	125.435	14.808	42.583	1.00	26.38	D
	ATOM	8118	O	ASP	D	579	124.715	15.590	43.200	1.00	25.82	D
	ATOM	8119	N	HIS	D	580	126.148	15.172	41.513	1.00	28.39	D
	ATOM	8120	CA	HIS	D	580	126.145	16.555	41.028	1.00	31.78	D
	ATOM	8121	CB	HIS	D	580	127.029	16.692	39.794	1.00	33.03	D
25	ATOM	8122	CG	HIS	D	580	126.607	15.830	38.654	1.00	37.41	D
	ATOM	8123	CD2	HIS	D	580	125.611	15.973	37.750	1.00	38.10	D
	ATOM	8124	ND1	HIS	D	580	127.244	14.648	38.342	1.00	39.09	D
	ATOM	8125	CE1	HIS	D	580	126.660	14.102	37.292	1.00	38.85	D
	ATOM	8126	NE2	HIS	D	580	125.666	14.885	36.913	1.00	39.22	D
30	ATOM	8127	C	HIS	D	580	124.745	17.113	40.723	1.00	33.01	D
	ATOM	8128	O	HIS	D	580	124.484	18.313	40.890	1.00	34.71	D
	ATOM	8129	N	GLU	D	581	123.836	16.251	40.292	1.00	33.24	D
	ATOM	8130	CA	GLU	D	581	122.486	16.693	39.995	1.00	32.71	D
	ATOM	8131	CB	GLU	D	581	121.700	15.544	39.375	1.00	35.03	D
35	ATOM	8132	CG	GLU	D	581	120.463	15.978	38.652	1.00	39.07	D
	ATOM	8133	CD	GLU	D	581	119.702	14.818	38.092	1.00	41.55	D
	ATOM	8134	OE1	GLU	D	581	120.332	14.026	37.350	1.00	43.80	D
	ATOM	8135	OE2	GLU	D	581	118.485	14.712	38.394	1.00	41.52	D
	ATOM	8136	C	GLU	D	581	121.788	17.202	41.266	1.00	31.80	D
40	ATOM	8137	O	GLU	D	581	121.244	18.306	41.260	1.00	31.97	D
	ATOM	8138	N	ARG	D	582	121.808	16.414	42.348	1.00	29.57	D
	ATOM	8139	CA	ARG	D	582	121.177	16.825	43.616	1.00	29.36	D
	ATOM	8140	CB	ARG	D	582	120.622	15.607	44.390	1.00	26.09	D
	ATOM	8141	CG	ARG	D	582	119.558	14.822	43.650	1.00	22.04	D
45	ATOM	8142	CD	ARG	D	582	118.850	13.766	44.496	1.00	20.11	D
	ATOM	8143	NE	ARG	D	582	118.024	12.908	43.636	1.00	19.38	D
	ATOM	8144	CZ	ARG	D	582	118.506	12.137	42.658	1.00	20.74	D
	ATOM	8145	NH1	ARG	D	582	119.808	12.105	42.415	1.00	22.11	D
	ATOM	8146	NH2	ARG	D	582	117.695	11.398	41.908	1.00	19.51	D
50	ATOM	8147	C	ARG	D	582	122.160	17.598	44.531	1.00	31.40	D
	ATOM	8148	O	ARG	D	582	121.796	18.063	45.622	1.00	29.69	D
	ATOM	8149	N	LYS	D	583	123.401	17.747	44.074	1.00	33.89	D
	ATOM	8150	CA	LYS	D	583	124.433	18.436	44.849	1.00	35.05	D
	ATOM	8151	CB	LYS	D	583	124.069	19.912	45.068	1.00	38.08	D

	ATOM	8152	CG	LYS	D	583	124.348	20.830	43.882	1.00	40.35	D
	ATOM	8153	CD	LYS	D	583	125.842	20.963	43.611	1.00	42.80	D
	ATOM	8154	CE	LYS	D	583	126.103	21.734	42.310	1.00	42.80	D
	ATOM	8155	NZ	LYS	D	583	125.618	23.153	42.366	1.00	43.25	D
5	ATOM	8156	C	LYS	D	583	124.627	17.755	46.202	1.00	34.05	D
	ATOM	8157	O	LYS	D	583	124.524	18.401	47.241	1.00	35.02	D
	ATOM	8158	N	ARG	D	584	124.898	16.449	46.172	1.00	33.23	D
	ATOM	8159	CA	ARG	D	584	125.128	15.634	47.370	1.00	31.46	D
	ATOM	8160	CB	ARG	D	584	123.854	14.861	47.768	1.00	29.44	D
10	ATOM	8161	CG	ARG	D	584	122.595	15.702	47.938	1.00	30.45	D
	ATOM	8162	CD	ARG	D	584	121.369	14.815	48.175	1.00	30.86	D
	ATOM	8163	NE	ARG	D	584	120.098	15.542	48.113	1.00	31.46	D
	ATOM	8164	CZ	ARG	D	584	118.904	14.965	48.229	1.00	32.25	D
	ATOM	8165	NH1	ARG	D	584	118.820	13.653	48.414	1.00	29.52	D
15	ATOM	8166	NH2	ARG	D	584	117.793	15.697	48.156	1.00	30.64	D
	ATOM	8167	C	ARG	D	584	126.247	14.622	47.065	1.00	31.14	D
	ATOM	8168	O	ARG	D	584	126.668	14.466	45.916	1.00	30.87	D
	ATOM	8169	N	CYS	D	585	126.732	13.961	48.111	1.00	30.50	D
	ATOM	8170	CA	CYS	D	585	127.762	12.937	48.009	1.00	29.49	D
20	ATOM	8171	CB	CYS	D	585	129.086	13.427	48.598	1.00	32.51	D
	ATOM	8172	SG	CYS	D	585	130.268	12.081	49.098	1.00	36.50	D
	ATOM	8173	C	CYS	D	585	127.298	11.719	48.809	1.00	28.24	D
	ATOM	8174	O	CYS	D	585	126.814	11.850	49.943	1.00	28.12	D
	ATOM	8175	N	ILE	D	586	127.434	10.546	48.193	1.00	25.25	D
25	ATOM	8176	CA	ILE	D	586	127.094	9.266	48.806	1.00	22.27	D
	ATOM	8177	CB	ILE	D	586	126.394	8.304	47.804	1.00	21.75	D
	ATOM	8178	CG2	ILE	D	586	126.164	6.967	48.464	1.00	18.50	D
	ATOM	8179	CG1	ILE	D	586	125.070	8.900	47.279	1.00	21.75	D
	ATOM	8180	CD1	ILE	D	586	125.217	9.902	46.122	1.00	19.83	D
30	ATOM	8181	C	ILE	D	586	128.460	8.670	49.123	1.00	22.41	D
	ATOM	8182	O	ILE	D	586	129.400	8.875	48.359	1.00	24.24	D
	ATOM	8183	N	SER	D	587	128.586	7.955	50.236	1.00	21.77	D
	ATOM	8184	CA	SER	D	587	129.856	7.319	50.595	1.00	19.65	D
	ATOM	8185	CB	SER	D	587	130.644	8.217	51.548	1.00	18.81	D
35	ATOM	8186	OG	SER	D	587	129.942	8.436	52.758	1.00	17.09	D
	ATOM	8187	C	SER	D	587	129.579	5.968	51.255	1.00	19.73	D
	ATOM	8188	O	SER	D	587	128.676	5.867	52.082	1.00	20.77	D
	ATOM	8189	N	ALA	D	588	130.334	4.936	50.874	1.00	19.14	D
	ATOM	8190	CA	ALA	D	588	130.169	3.595	51.436	1.00	18.83	D
40	ATOM	8191	CB	ALA	D	588	129.817	2.586	50.342	1.00	17.57	D
	ATOM	8192	C	ALA	D	588	131.483	3.220	52.105	1.00	18.48	D
	ATOM	8193	O	ALA	D	588	132.549	3.280	51.482	1.00	18.12	D
	ATOM	8194	N	SER	D	589	131.387	2.829	53.375	1.00	19.29	D
	ATOM	8195	CA	SER	D	589	132.546	2.500	54.224	1.00	20.33	D
45	ATOM	8196	CB	SER	D	589	132.552	3.487	55.416	1.00	21.31	D
	ATOM	8197	OG	SER	D	589	133.427	3.106	56.474	1.00	19.54	D
	ATOM	8198	C	SER	D	589	132.633	1.058	54.749	1.00	20.03	D
	ATOM	8199	O	SER	D	589	131.638	0.322	54.743	1.00	20.59	D
	ATOM	8200	N	MSE	D	590	133.837	0.677	55.189	1.00	22.56	D
50	ATOM	8201	CA	MSE	D	590	134.089	-0.644	55.760	1.00	25.48	D
	ATOM	8202	CB	MSE	D	590	135.578	-0.827	56.067	1.00	28.07	D
	ATOM	8203	CG	MSE	D	590	135.932	-2.225	56.531	1.00	30.40	D
	ATOM	8204	SE	MSE	D	590	137.843	-2.501	56.672	1.00	39.74	D
	ATOM	8205	CE	MSE	D	590	138.123	-3.610	55.120	1.00	33.01	D

	ATOM	8206	C	MSE	D	590	133.271	-0.777	57.053	1.00	26.26	D
	ATOM	8207	O	MSE	D	590	133.045	-1.883	57.540	1.00	27.96	D
	ATOM	8208	N	ASP	D	591	132.806	0.352	57.587	1.00	24.74	D
	ATOM	8209	CA	ASP	D	591	131.999	0.333	58.790	1.00	24.47	D
5	ATOM	8210	CB	ASP	D	591	131.931	1.722	59.447	1.00	25.09	D
	ATOM	8211	CG	ASP	D	591	131.115	2.730	58.635	1.00	26.02	D
	ATOM	8212	OD1	ASP	D	591	130.116	2.338	57.987	1.00	23.16	D
	ATOM	8213	OD2	ASP	D	591	131.461	3.930	58.668	1.00	28.61	D
	ATOM	8214	C	ASP	D	591	130.575	-0.167	58.535	1.00	25.63	D
10	ATOM	8215	O	ASP	D	591	129.731	-0.111	59.435	1.00	27.48	D
	ATOM	8216	N	THR	D	592	130.280	-0.612	57.315	1.00	24.13	D
	ATOM	8217	CA	THR	D	592	128.953	-1.144	57.027	1.00	23.60	D
	ATOM	8218	CB	THR	D	592	128.479	-2.010	58.217	1.00	23.93	D
	ATOM	8219	OG1	THR	D	592	129.276	-3.197	58.290	1.00	24.58	D
15	ATOM	8220	CG2	THR	D	592	127.032	-2.388	58.071	1.00	25.94	D
	ATOM	8221	C	THR	D	592	127.858	-0.117	56.694	1.00	23.10	D
	ATOM	8222	O	THR	D	592	126.814	-0.466	56.131	1.00	23.01	D
	ATOM	8223	N	THR	D	593	128.086	1.146	57.020	1.00	21.17	D
	ATOM	8224	CA	THR	D	593	127.084	2.164	56.743	1.00	20.07	D
20	ATOM	8225	CB	THR	D	593	127.097	3.238	57.829	1.00	19.96	D
	ATOM	8226	OG1	THR	D	593	128.317	3.981	57.736	1.00	20.19	D
	ATOM	8227	CG2	THR	D	593	127.012	2.601	59.205	1.00	20.49	D
	ATOM	8228	C	THR	D	593	127.303	2.861	55.400	1.00	20.54	D
	ATOM	8229	O	THR	D	593	128.282	2.602	54.705	1.00	20.50	D
25	ATOM	8230	N	ILE	D	594	126.360	3.728	55.039	1.00	19.85	D
	ATOM	8231	CA	ILE	D	594	126.422	4.520	53.823	1.00	18.48	D
	ATOM	8232	CB	ILE	D	594	125.423	4.012	52.749	1.00	17.96	D
	ATOM	8233	CG2	ILE	D	594	125.476	4.931	51.512	1.00	16.27	D
	ATOM	8234	CG1	ILE	D	594	125.763	2.564	52.352	1.00	17.94	D
30	ATOM	8235	CD1	ILE	D	594	124.874	1.976	51.244	1.00	13.75	D
	ATOM	8236	C	ILE	D	594	126.013	5.920	54.297	1.00	20.05	D
	ATOM	8237	O	ILE	D	594	125.125	6.060	55.147	1.00	19.44	D
	ATOM	8238	N	ARG	D	595	126.661	6.961	53.787	1.00	21.73	D
	ATOM	8239	CA	ARG	D	595	126.294	8.304	54.229	1.00	24.25	D
35	ATOM	8240	CB	ARG	D	595	127.380	8.898	55.133	1.00	26.38	D
	ATOM	8241	CG	ARG	D	595	127.485	8.261	56.508	1.00	27.19	D
	ATOM	8242	CD	ARG	D	595	128.489	9.003	57.373	1.00	29.27	D
	ATOM	8243	NE	ARG	D	595	128.184	8.848	58.797	1.00	33.82	D
	ATOM	8244	CZ	ARG	D	595	128.465	9.753	59.732	1.00	34.00	D
40	ATOM	8245	NH1	ARG	D	595	129.068	10.889	59.398	1.00	34.40	D
	ATOM	8246	NH2	ARG	D	595	128.125	9.528	60.998	1.00	33.02	D
	ATOM	8247	C	ARG	D	595	125.999	9.282	53.108	1.00	24.90	D
	ATOM	8248	O	ARG	D	595	126.702	9.329	52.102	1.00	25.43	D
	ATOM	8249	N	ILE	D	596	124.939	10.056	53.294	1.00	25.81	D
45	ATOM	8250	CA	ILE	D	596	124.540	11.056	52.319	1.00	27.39	D
	ATOM	8251	CB	ILE	D	596	123.000	11.093	52.138	1.00	27.40	D
	ATOM	8252	CG2	ILE	D	596	122.646	11.950	50.935	1.00	27.77	D
	ATOM	8253	CG1	ILE	D	596	122.459	9.681	51.891	1.00	27.13	D
	ATOM	8254	CD1	ILE	D	596	122.953	9.062	50.590	1.00	26.64	D
50	ATOM	8255	C	ILE	D	596	125.013	12.392	52.870	1.00	28.16	D
	ATOM	8256	O	ILE	D	596	124.637	12.787	53.976	1.00	28.61	D
	ATOM	8257	N	TRP	D	597	125.862	13.078	52.118	1.00	28.67	D
	ATOM	8258	CA	TRP	D	597	126.368	14.368	52.568	1.00	28.04	D
	ATOM	8259	CB	TRP	D	597	127.893	14.391	52.515	1.00	29.61	D

	ATOM	8260	CG	TRP	D	597	128.562	13.228	53.155	1.00	28.57	D
	ATOM	8261	CD2	TRP	D	597	129.116	13.186	54.470	1.00	27.43	D
	ATOM	8262	CE2	TRP	D	597	129.707	11.918	54.634	1.00	27.37	D
	ATOM	8263	CE3	TRP	D	597	129.172	14.103	55.529	1.00	27.46	D
5	ATOM	8264	CD1	TRP	D	597	128.822	12.016	52.589	1.00	29.00	D
	ATOM	8265	NE1	TRP	D	597	129.516	11.221	53.469	1.00	27.32	D
	ATOM	8266	CZ2	TRP	D	597	130.349	11.541	55.817	1.00	27.76	D
	ATOM	8267	CZ3	TRP	D	597	129.810	13.729	56.703	1.00	27.02	D
	ATOM	8268	CH2	TRP	D	597	130.389	12.457	56.838	1.00	27.58	D
10	ATOM	8269	C	TRP	D	597	125.838	15.486	51.684	1.00	27.75	D
	ATOM	8270	O	TRP	D	597	125.729	15.326	50.472	1.00	27.73	D
	ATOM	8271	N	ASP	D	598	125.519	16.624	52.284	1.00	28.69	D
	ATOM	8272	CA	ASP	D	598	125.012	17.773	51.527	1.00	29.82	D
	ATOM	8273	CB	ASP	D	598	123.966	18.511	52.381	1.00	29.96	D
15	ATOM	8274	CG	ASP	D	598	123.483	19.816	51.749	1.00	30.01	D
	ATOM	8275	OD1	ASP	D	598	123.889	20.118	50.601	1.00	29.40	D
	ATOM	8276	OD2	ASP	D	598	122.700	20.537	52.417	1.00	28.15	D
	ATOM	8277	C	ASP	D	598	126.197	18.694	51.177	1.00	28.75	D
	ATOM	8278	O	ASP	D	598	126.880	19.192	52.067	1.00	26.58	D
20	ATOM	8279	N	LEU	D	599	126.442	18.912	49.884	1.00	29.62	D
	ATOM	8280	CA	LEU	D	599	127.567	19.753	49.466	1.00	32.72	D
	ATOM	8281	CB	LEU	D	599	128.148	19.244	48.141	1.00	30.82	D
	ATOM	8282	CG	LEU	D	599	128.646	17.780	48.141	1.00	31.03	D
	ATOM	8283	CD1	LEU	D	599	129.360	17.472	46.822	1.00	29.75	D
25	ATOM	8284	CD2	LEU	D	599	129.579	17.529	49.309	1.00	28.77	D
	ATOM	8285	C	LEU	D	599	127.238	21.246	49.383	1.00	35.04	D
	ATOM	8286	O	LEU	D	599	127.899	22.009	48.686	1.00	34.05	D
	ATOM	8287	N	GLU	D	600	126.228	21.651	50.145	1.00	39.89	D
	ATOM	8288	CA	GLU	D	600	125.793	23.041	50.205	1.00	42.71	D
30	ATOM	8289	CB	GLU	D	600	124.279	23.118	49.998	1.00	43.83	D
	ATOM	8290	CG	GLU	D	600	123.818	22.578	48.659	1.00	49.15	D
	ATOM	8291	CD	GLU	D	600	124.057	23.565	47.524	1.00	52.47	D
	ATOM	8292	OE1	GLU	D	600	123.836	23.205	46.340	1.00	54.37	D
	ATOM	8293	OE2	GLU	D	600	124.462	24.710	47.820	1.00	53.81	D
35	ATOM	8294	C	GLU	D	600	126.154	23.614	51.581	1.00	43.08	D
	ATOM	8295	O	GLU	D	600	125.956	24.799	51.847	1.00	44.92	D
	ATOM	8296	N	ASN	D	605	126.681	22.769	52.461	1.00	42.60	D
	ATOM	8297	CA	ASN	D	605	127.049	23.217	53.798	1.00	41.25	D
	ATOM	8298	CB	ASN	D	605	125.787	23.392	54.640	1.00	41.21	D
40	ATOM	8299	CG	ASN	D	605	125.003	22.105	54.794	1.00	42.82	D
	ATOM	8300	OD1	ASN	D	605	124.753	21.383	53.830	1.00	41.44	D
	ATOM	8301	ND2	ASN	D	605	124.599	21.819	56.024	1.00	44.97	D
	ATOM	8302	C	ASN	D	605	128.006	22.222	54.440	1.00	40.16	D
	ATOM	8303	O	ASN	D	605	128.507	22.442	55.544	1.00	39.89	D
45	ATOM	8304	N	GLY	D	606	128.259	21.135	53.712	1.00	39.38	D
	ATOM	8305	CA	GLY	D	606	129.165	20.091	54.156	1.00	36.83	D
	ATOM	8306	C	GLY	D	606	128.629	19.279	55.311	1.00	35.89	D
	ATOM	8307	O	GLY	D	606	129.336	18.446	55.865	1.00	35.05	D
	ATOM	8308	N	GLU	D	607	127.378	19.523	55.675	1.00	35.04	D
50	ATOM	8309	CA	GLU	D	607	126.771	18.814	56.779	1.00	35.34	D
	ATOM	8310	CB	GLU	D	607	125.624	19.635	57.350	1.00	38.59	D
	ATOM	8311	CG	GLU	D	607	126.032	20.652	58.401	1.00	44.13	D
	ATOM	8312	CD	GLU	D	607	124.828	21.150	59.183	1.00	49.69	D
	ATOM	8313	OE1	GLU	D	607	124.093	20.289	59.749	1.00	51.01	D

	ATOM	8314	OE2	GLU	D	607	124.608	22.394	59.227	1.00	52.33	D
	ATOM	8315	C	GLU	D	607	126.271	17.415	56.411	1.00	33.71	D
	ATOM	8316	O	GLU	D	607	125.991	17.144	55.247	1.00	33.25	D
	ATOM	8317	N	LEU	D	608	126.175	16.521	57.397	1.00	31.85	D
5	ATOM	8318	CA	LEU	D	608	125.686	15.175	57.125	1.00	30.51	D
	ATOM	8319	CB	LEU	D	608	126.052	14.216	58.253	1.00	27.96	D
	ATOM	8320	CG	LEU	D	608	125.557	12.778	58.041	1.00	28.56	D
	ATOM	8321	CD1	LEU	D	608	126.456	12.051	57.046	1.00	24.69	D
	ATOM	8322	CD2	LEU	D	608	125.531	12.032	59.394	1.00	28.82	D
10	ATOM	8323	C	LEU	D	608	124.169	15.253	56.971	1.00	30.57	D
	ATOM	8324	O	LEU	D	608	123.532	16.124	57.573	1.00	31.18	D
	ATOM	8325	N	MSE	D	625	123.605	14.363	56.150	1.00	29.87	D
	ATOM	8326	CA	MSE	D	625	122.153	14.303	55.888	1.00	30.31	D
	ATOM	8327	CB	MSE	D	625	121.846	14.367	54.381	1.00	31.08	D
15	ATOM	8328	CG	MSE	D	625	122.016	15.737	53.754	1.00	33.02	D
	ATOM	8329	SE	MSE	D	625	121.598	15.802	51.862	1.00	38.72	D
	ATOM	8330	CE	MSE	D	625	119.705	15.354	51.962	1.00	32.55	D
	ATOM	8331	C	MSE	D	625	121.523	13.022	56.410	1.00	27.88	D
	ATOM	8332	O	MSE	D	625	120.538	13.032	57.145	1.00	28.06	D
20	ATOM	8333	N	TYR	D	626	122.073	11.901	55.993	1.00	25.99	D
	ATOM	8334	CA	TYR	D	626	121.505	10.670	56.444	1.00	24.99	D
	ATOM	8335	CB	TYR	D	626	120.453	10.176	55.461	1.00	25.25	D
	ATOM	8336	CG	TYR	D	626	119.434	11.186	54.999	1.00	24.62	D
	ATOM	8337	CD1	TYR	D	626	118.409	11.612	55.842	1.00	21.86	D
25	ATOM	8338	CE1	TYR	D	626	117.391	12.424	55.363	1.00	23.49	D
	ATOM	8339	CD2	TYR	D	626	119.426	11.615	53.669	1.00	24.69	D
	ATOM	8340	CE2	TYR	D	626	118.421	12.421	53.179	1.00	24.51	D
	ATOM	8341	CZ	TYR	D	626	117.396	12.820	54.023	1.00	24.72	D
	ATOM	8342	OH	TYR	D	626	116.346	13.555	53.502	1.00	25.76	D
30	ATOM	8343	C	TYR	D	626	122.555	9.597	56.565	1.00	23.88	D
	ATOM	8344	O	TYR	D	626	123.605	9.652	55.923	1.00	23.89	D
	ATOM	8345	N	THR	D	627	122.255	8.616	57.406	1.00	23.42	D
	ATOM	8346	CA	THR	D	627	123.122	7.472	57.564	1.00	20.62	D
	ATOM	8347	CB	THR	D	627	123.589	7.271	58.987	1.00	19.43	D
35	ATOM	8348	OG1	THR	D	627	124.268	8.447	59.440	1.00	20.14	D
	ATOM	8349	CG2	THR	D	627	124.535	6.066	59.050	1.00	17.31	D
	ATOM	8350	C	THR	D	627	122.235	6.308	57.191	1.00	19.41	D
	ATOM	8351	O	THR	D	627	121.244	6.050	57.859	1.00	18.63	D
	ATOM	8352	N	LEU	D	628	122.577	5.640	56.095	1.00	19.47	D
40	ATOM	8353	CA	LEU	D	628	121.821	4.485	55.626	1.00	19.11	D
	ATOM	8354	CB	LEU	D	628	121.755	4.469	54.108	1.00	17.80	D
	ATOM	8355	CG	LEU	D	628	121.117	5.669	53.396	1.00	16.59	D
	ATOM	8356	CD1	LEU	D	628	121.092	5.364	51.890	1.00	16.34	D
	ATOM	8357	CD2	LEU	D	628	119.712	5.929	53.916	1.00	13.86	D
45	ATOM	8358	C	LEU	D	628	122.523	3.227	56.111	1.00	19.57	D
	ATOM	8359	O	LEU	D	628	123.674	2.966	55.744	1.00	20.61	D
	ATOM	8360	N	GLN	D	629	121.817	2.456	56.936	1.00	19.21	D
	ATOM	8361	CA	GLN	D	629	122.331	1.216	57.512	1.00	19.59	D
	ATOM	8362	CB	GLN	D	629	122.142	1.262	59.031	1.00	18.99	D
50	ATOM	8363	CG	GLN	D	629	122.640	0.047	59.795	1.00	19.95	D
	ATOM	8364	CD	GLN	D	629	124.155	-0.088	59.756	1.00	21.73	D
	ATOM	8365	OE1	GLN	D	629	124.709	-0.697	58.841	1.00	21.66	D
	ATOM	8366	NE2	GLN	D	629	124.834	0.492	60.751	1.00	21.48	D
	ATOM	8367	C	GLN	D	629	121.565	0.034	56.922	1.00	19.26	D

	ATOM	8368	O	GLN	D	629	120.435	-0.224	57.313	1.00	22.24	D
	ATOM	8369	N	GLY	D	630	122.178	-0.689	55.993	1.00	18.64	D
	ATOM	8370	CA	GLY	D	630	121.480	-1.802	55.386	1.00	19.70	D
	ATOM	8371	C	GLY	D	630	122.361	-2.917	54.860	1.00	21.44	D
5	ATOM	8372	O	GLY	D	630	122.068	-3.533	53.844	1.00	22.81	D
	ATOM	8373	N	HIS	D	631	123.459	-3.179	55.544	1.00	22.39	D
	ATOM	8374	CA	HIS	D	631	124.368	-4.236	55.143	1.00	23.12	D
	ATOM	8375	CB	HIS	D	631	125.425	-3.720	54.169	1.00	26.25	D
	ATOM	8376	CG	HIS	D	631	124.856	-3.144	52.915	1.00	28.65	D
10	ATOM	8377	CD2	HIS	D	631	124.544	-1.870	52.586	1.00	28.78	D
	ATOM	8378	ND1	HIS	D	631	124.504	-3.920	51.833	1.00	29.43	D
	ATOM	8379	CE1	HIS	D	631	124.002	-3.146	50.887	1.00	28.34	D
	ATOM	8380	NE2	HIS	D	631	124.015	-1.898	51.319	1.00	28.49	D
	ATOM	8381	C	HIS	D	631	125.030	-4.618	56.440	1.00	22.81	D
15	ATOM	8382	O	HIS	D	631	125.008	-3.860	57.402	1.00	25.35	D
	ATOM	8383	N	THR	D	632	125.661	-5.774	56.455	1.00	21.41	D
	ATOM	8384	CA	THR	D	632	126.288	-6.261	57.663	1.00	20.28	D
	ATOM	8385	CB	THR	D	632	125.646	-7.591	58.047	1.00	18.49	D
	ATOM	8386	OG1	THR	D	632	125.767	-8.524	56.957	1.00	18.30	D
20	ATOM	8387	CG2	THR	D	632	124.173	-7.371	58.349	1.00	13.99	D
	ATOM	8388	C	THR	D	632	127.771	-6.466	57.509	1.00	20.33	D
	ATOM	8389	O	THR	D	632	128.427	-6.983	58.405	1.00	22.76	D
	ATOM	8390	N	ALA	D	633	128.291	-6.053	56.367	1.00	19.78	D
	ATOM	8391	CA	ALA	D	633	129.695	-6.224	56.061	1.00	18.83	D
25	ATOM	8392	CB	ALA	D	633	129.877	-7.469	55.239	1.00	17.26	D
	ATOM	8393	C	ALA	D	633	130.169	-5.029	55.282	1.00	19.55	D
	ATOM	8394	O	ALA	D	633	129.385	-4.126	54.991	1.00	19.68	D
	ATOM	8395	N	LEU	D	634	131.455	-5.024	54.951	1.00	20.72	D
	ATOM	8396	CA	LEU	D	634	132.051	-3.944	54.175	1.00	20.81	D
30	ATOM	8397	CB	LEU	D	634	133.478	-4.347	53.790	1.00	21.47	D
	ATOM	8398	CG	LEU	D	634	134.286	-3.752	52.639	1.00	22.59	D
	ATOM	8399	CD1	LEU	D	634	133.982	-4.534	51.395	1.00	25.22	D
	ATOM	8400	CD2	LEU	D	634	133.968	-2.263	52.448	1.00	26.73	D
	ATOM	8401	C	LEU	D	634	131.211	-3.634	52.940	1.00	21.70	D
35	ATOM	8402	O	LEU	D	634	130.889	-4.523	52.138	1.00	22.37	D
	ATOM	8403	N	VAL	D	635	130.822	-2.371	52.807	1.00	21.89	D
	ATOM	8404	CA	VAL	D	635	130.038	-1.957	51.646	1.00	23.38	D
	ATOM	8405	CB	VAL	D	635	128.929	-0.951	52.019	1.00	23.26	D
	ATOM	8406	CG1	VAL	D	635	128.136	-0.574	50.771	1.00	25.04	D
40	ATOM	8407	CG2	VAL	D	635	128.008	-1.545	53.048	1.00	21.55	D
	ATOM	8408	C	VAL	D	635	131.019	-1.303	50.670	1.00	24.61	D
	ATOM	8409	O	VAL	D	635	131.455	-0.164	50.878	1.00	22.67	D
	ATOM	8410	N	GLY	D	636	131.352	-2.036	49.607	1.00	25.64	D
	ATOM	8411	CA	GLY	D	636	132.320	-1.552	48.641	1.00	26.53	D
45	ATOM	8412	C	GLY	D	636	131.874	-1.151	47.254	1.00	26.66	D
	ATOM	8413	O	GLY	D	636	132.687	-0.595	46.509	1.00	27.11	D
	ATOM	8414	N	LEU	D	637	130.612	-1.418	46.906	1.00	26.43	D
	ATOM	8415	CA	LEU	D	637	130.077	-1.089	45.582	1.00	24.26	D
	ATOM	8416	CB	LEU	D	637	129.705	-2.367	44.825	1.00	22.49	D
50	ATOM	8417	CG	LEU	D	637	130.896	-3.277	44.542	1.00	21.34	D
	ATOM	8418	CD1	LEU	D	637	132.028	-2.399	44.003	1.00	18.59	D
	ATOM	8419	CD2	LEU	D	637	131.352	-3.982	45.809	1.00	23.19	D
	ATOM	8420	C	LEU	D	637	128.868	-0.163	45.606	1.00	25.18	D
	ATOM	8421	O	LEU	D	637	127.843	-0.503	46.182	1.00	26.31	D

	ATOM	8422	N	LEU	D	638	129.009	1.004	44.970	1.00	26.27	D
	ATOM	8423	CA	LEU	D	638	127.959	2.021	44.854	1.00	25.24	D
	ATOM	8424	CB	LEU	D	638	128.335	3.308	45.579	1.00	25.17	D
	ATOM	8425	CG	LEU	D	638	128.217	3.292	47.092	1.00	26.38	D
5	ATOM	8426	CD1	LEU	D	638	128.445	4.708	47.617	1.00	25.29	D
	ATOM	8427	CD2	LEU	D	638	126.827	2.778	47.484	1.00	23.90	D
	ATOM	8428	C	LEU	D	638	127.772	2.372	43.396	1.00	25.47	D
	ATOM	8429	O	LEU	D	638	128.746	2.427	42.638	1.00	24.74	D
	ATOM	8430	N	ARG	D	639	126.515	2.639	43.029	1.00	25.82	D
10	ATOM	8431	CA	ARG	D	639	126.101	2.999	41.661	1.00	24.67	D
	ATOM	8432	CB	ARG	D	639	125.735	1.733	40.875	1.00	24.23	D
	ATOM	8433	CG	ARG	D	639	126.472	1.524	39.569	1.00	24.13	D
	ATOM	8434	CD	ARG	D	639	127.923	1.341	39.843	1.00	24.24	D
	ATOM	8435	NE	ARG	D	639	128.539	0.275	39.061	1.00	25.29	D
15	ATOM	8436	CZ	ARG	D	639	129.345	0.488	38.027	1.00	26.83	D
	ATOM	8437	NH1	ARG	D	639	129.609	1.735	37.658	1.00	22.95	D
	ATOM	8438	NH2	ARG	D	639	129.909	-0.538	37.387	1.00	27.61	D
	ATOM	8439	C	ARG	D	639	124.857	3.877	41.777	1.00	24.76	D
	ATOM	8440	O	ARG	D	639	123.942	3.540	42.519	1.00	24.70	D
20	ATOM	8441	N	LEU	D	640	124.821	4.991	41.046	1.00	25.49	D
	ATOM	8442	CA	LEU	D	640	123.668	5.908	41.066	1.00	23.58	D
	ATOM	8443	CB	LEU	D	640	124.142	7.354	41.250	1.00	20.68	D
	ATOM	8444	CG	LEU	D	640	123.301	8.220	42.178	1.00	21.27	D
	ATOM	8445	CD1	LEU	D	640	123.483	9.698	41.849	1.00	19.99	D
25	ATOM	8446	CD2	LEU	D	640	121.854	7.834	42.058	1.00	21.23	D
	ATOM	8447	C	LEU	D	640	122.888	5.800	39.753	1.00	23.09	D
	ATOM	8448	O	LEU	D	640	123.464	5.886	38.677	1.00	25.33	D
	ATOM	8449	N	SER	D	641	121.582	5.598	39.846	1.00	22.47	D
	ATOM	8450	CA	SER	D	641	120.741	5.498	38.668	1.00	21.80	D
30	ATOM	8451	CB	SER	D	641	119.920	4.212	38.713	1.00	23.05	D
	ATOM	8452	OG	SER	D	641	118.628	4.399	38.170	1.00	26.20	D
	ATOM	8453	C	SER	D	641	119.837	6.712	38.706	1.00	22.79	D
	ATOM	8454	O	SER	D	641	119.697	7.344	39.743	1.00	21.44	D
	ATOM	8455	N	ASP	D	642	119.206	7.052	37.596	1.00	25.87	D
35	ATOM	8456	CA	ASP	D	642	118.361	8.230	37.631	1.00	29.02	D
	ATOM	8457	CB	ASP	D	642	117.753	8.507	36.258	1.00	32.11	D
	ATOM	8458	CG	ASP	D	642	117.066	9.854	36.206	1.00	35.97	D
	ATOM	8459	OD1	ASP	D	642	117.782	10.877	36.333	1.00	38.30	D
	ATOM	8460	OD2	ASP	D	642	115.817	9.904	36.059	1.00	37.81	D
40	ATOM	8461	C	ASP	D	642	117.247	8.077	38.655	1.00	28.71	D
	ATOM	8462	O	ASP	D	642	116.649	9.055	39.098	1.00	28.83	D
	ATOM	8463	N	LYS	D	643	116.975	6.847	39.047	1.00	29.24	D
	ATOM	8464	CA	LYS	D	643	115.903	6.626	39.989	1.00	29.96	D
	ATOM	8465	CB	LYS	D	643	114.760	5.934	39.241	1.00	31.36	D
45	ATOM	8466	CG	LYS	D	643	113.626	5.382	40.076	1.00	36.57	D
	ATOM	8467	CD	LYS	D	643	112.491	4.792	39.183	1.00	38.95	D
	ATOM	8468	CE	LYS	D	643	111.899	5.844	38.222	1.00	40.27	D
	ATOM	8469	NZ	LYS	D	643	110.719	5.330	37.453	1.00	40.99	D
	ATOM	8470	C	LYS	D	643	116.325	5.831	41.222	1.00	29.02	D
50	ATOM	8471	O	LYS	D	643	115.628	5.832	42.234	1.00	29.30	D
	ATOM	8472	N	PHE	D	644	117.483	5.187	41.160	1.00	27.45	D
	ATOM	8473	CA	PHE	D	644	117.924	4.370	42.276	1.00	25.90	D
	ATOM	8474	CB	PHE	D	644	117.822	2.889	41.918	1.00	23.62	D
	ATOM	8475	CG	PHE	D	644	116.428	2.416	41.670	1.00	22.94	D

	ATOM	8476	CD1	PHE	D	644	116.097	1.784	40.480	1.00	23.53	D
	ATOM	8477	CD2	PHE	D	644	115.448	2.567	42.632	1.00	21.03	D
	ATOM	8478	CE1	PHE	D	644	114.807	1.309	40.266	1.00	21.81	D
	ATOM	8479	CE2	PHE	D	644	114.164	2.094	42.416	1.00	18.29	D
5	ATOM	8480	CZ	PHE	D	644	113.847	1.467	41.237	1.00	17.27	D
	ATOM	8481	C	PHE	D	644	119.337	4.618	42.735	1.00	26.43	D
	ATOM	8482	O	PHE	D	644	120.164	5.136	41.989	1.00	25.68	D
	ATOM	8483	N	LEU	D	645	119.589	4.238	43.988	1.00	27.14	D
	ATOM	8484	CA	LEU	D	645	120.911	4.318	44.608	1.00	26.31	D
10	ATOM	8485	CB	LEU	D	645	120.914	5.234	45.828	1.00	27.08	D
	ATOM	8486	CG	LEU	D	645	122.217	5.194	46.640	1.00	27.94	D
	ATOM	8487	CD1	LEU	D	645	123.290	5.975	45.918	1.00	29.78	D
	ATOM	8488	CD2	LEU	D	645	121.994	5.766	48.028	1.00	27.68	D
	ATOM	8489	C	LEU	D	645	121.152	2.890	45.059	1.00	24.69	D
15	ATOM	8490	O	LEU	D	645	120.758	2.514	46.146	1.00	26.35	D
	ATOM	8491	N	VAL	D	646	121.786	2.100	44.206	1.00	23.16	D
	ATOM	8492	CA	VAL	D	646	122.056	0.706	44.499	1.00	21.12	D
	ATOM	8493	CB	VAL	D	646	122.116	-0.101	43.212	1.00	20.50	D
	ATOM	8494	CG1	VAL	D	646	122.047	-1.583	43.514	1.00	21.04	D
20	ATOM	8495	CG2	VAL	D	646	120.997	0.334	42.283	1.00	20.61	D
	ATOM	8496	C	VAL	D	646	123.384	0.523	45.211	1.00	20.80	D
	ATOM	8497	O	VAL	D	646	124.375	1.159	44.857	1.00	21.52	D
	ATOM	8498	N	SER	D	647	123.408	-0.356	46.208	1.00	20.76	D
	ATOM	8499	CA	SER	D	647	124.637	-0.643	46.936	1.00	19.72	D
25	ATOM	8500	CB	SER	D	647	124.706	0.166	48.231	1.00	19.38	D
	ATOM	8501	OG	SER	D	647	123.594	-0.100	49.071	1.00	20.83	D
	ATOM	8502	C	SER	D	647	124.723	-2.140	47.249	1.00	19.78	D
	ATOM	8503	O	SER	D	647	123.694	-2.816	47.373	1.00	18.23	D
	ATOM	8504	N	ALA	D	648	125.950	-2.654	47.344	1.00	18.94	D
30	ATOM	8505	CA	ALA	D	648	126.175	-4.060	47.646	1.00	19.09	D
	ATOM	8506	CB	ALA	D	648	126.463	-4.850	46.377	1.00	15.72	D
	ATOM	8507	C	ALA	D	648	127.337	-4.180	48.618	1.00	20.74	D
	ATOM	8508	O	ALA	D	648	128.279	-3.399	48.547	1.00	22.53	D
	ATOM	8509	N	ALA	D	649	127.253	-5.148	49.533	1.00	21.16	D
35	ATOM	8510	CA	ALA	D	649	128.301	-5.372	50.514	1.00	20.36	D
	ATOM	8511	CB	ALA	D	649	127.774	-5.097	51.911	1.00	23.59	D
	ATOM	8512	C	ALA	D	649	128.912	-6.772	50.457	1.00	20.64	D
	ATOM	8513	O	ALA	D	649	128.453	-7.663	49.723	1.00	19.52	D
	ATOM	8514	N	ALA	D	650	129.951	-6.944	51.271	1.00	18.79	D
40	ATOM	8515	CA	ALA	D	650	130.703	-8.192	51.372	1.00	17.83	D
	ATOM	8516	CB	ALA	D	650	131.839	-8.012	52.334	1.00	17.25	D
	ATOM	8517	C	ALA	D	650	129.889	-9.409	51.786	1.00	17.38	D
	ATOM	8518	O	ALA	D	650	130.337	-10.545	51.626	1.00	16.75	D
	ATOM	8519	N	ASP	D	651	128.699	-9.190	52.329	1.00	18.32	D
45	ATOM	8520	CA	ASP	D	651	127.880	-10.323	52.748	1.00	19.29	D
	ATOM	8521	CB	ASP	D	651	126.982	-9.930	53.920	1.00	21.96	D
	ATOM	8522	CG	ASP	D	651	126.027	-8.804	53.568	1.00	26.40	D
	ATOM	8523	OD1	ASP	D	651	125.508	-8.816	52.425	1.00	28.33	D
	ATOM	8524	OD2	ASP	D	651	125.781	-7.924	54.436	1.00	25.72	D
50	ATOM	8525	C	ASP	D	651	127.026	-10.856	51.609	1.00	19.07	D
	ATOM	8526	O	ASP	D	651	126.244	-11.789	51.787	1.00	20.37	D
	ATOM	8527	N	GLY	D	652	127.164	-10.256	50.437	1.00	19.11	D
	ATOM	8528	CA	GLY	D	652	126.370	-10.711	49.315	1.00	18.71	D
	ATOM	8529	C	GLY	D	652	125.024	-10.018	49.213	1.00	18.78	D

	ATOM	8530	O	GLY	D	652	124.142	-10.475	48.479	1.00	17.99	D
	ATOM	8531	N	SER	D	653	124.841	-8.926	49.950	1.00	20.24	D
	ATOM	8532	CA	SER	D	653	123.575	-8.198	49.864	1.00	21.58	D
	ATOM	8533	CB	SER	D	653	123.133	-7.678	51.236	1.00	21.54	D
5	ATOM	8534	OG	SER	D	653	124.037	-6.731	51.772	1.00	22.98	D
	ATOM	8535	C	SER	D	653	123.665	-7.033	48.881	1.00	22.14	D
	ATOM	8536	O	SER	D	653	124.742	-6.510	48.598	1.00	21.79	D
	ATOM	8537	N	ILE	D	654	122.515	-6.652	48.350	1.00	23.25	D
	ATOM	8538	CA	ILE	D	654	122.418	-5.554	47.409	1.00	25.80	D
10	ATOM	8539	CB	ILE	D	654	122.165	-6.055	45.982	1.00	26.21	D
	ATOM	8540	CG2	ILE	D	654	122.297	-4.918	45.003	1.00	26.27	D
	ATOM	8541	CG1	ILE	D	654	123.154	-7.158	45.616	1.00	28.16	D
	ATOM	8542	CD1	ILE	D	654	122.870	-7.785	44.254	1.00	28.37	D
	ATOM	8543	C	ILE	D	654	121.197	-4.754	47.836	1.00	26.75	D
15	ATOM	8544	O	ILE	D	654	120.122	-5.323	48.064	1.00	27.01	D
	ATOM	8545	N	ARG	D	655	121.346	-3.443	47.951	1.00	27.07	D
	ATOM	8546	CA	ARG	D	655	120.216	-2.626	48.356	1.00	27.67	D
	ATOM	8547	CB	ARG	D	655	120.467	-2.029	49.737	1.00	28.04	D
	ATOM	8548	CG	ARG	D	655	120.592	-3.062	50.832	1.00	29.00	D
20	ATOM	8549	CD	ARG	D	655	119.901	-2.605	52.103	1.00	31.71	D
	ATOM	8550	NE	ARG	D	655	118.574	-3.199	52.240	1.00	33.84	D
	ATOM	8551	CZ	ARG	D	655	118.328	-4.314	52.914	1.00	33.80	D
	ATOM	8552	NH1	ARG	D	655	119.314	-4.960	53.527	1.00	33.02	D
	ATOM	8553	NH2	ARG	D	655	117.094	-4.787	52.953	1.00	36.00	D
25	ATOM	8554	C	ARG	D	655	119.903	-1.524	47.358	1.00	27.31	D
	ATOM	8555	O	ARG	D	655	120.797	-0.985	46.706	1.00	26.04	D
	ATOM	8556	N	GLY	D	656	118.620	-1.203	47.237	1.00	27.56	D
	ATOM	8557	CA	GLY	D	656	118.206	-0.164	46.315	1.00	28.15	D
	ATOM	8558	C	GLY	D	656	117.482	0.916	47.087	1.00	27.66	D
30	ATOM	8559	O	GLY	D	656	116.514	0.621	47.775	1.00	28.41	D
	ATOM	8560	N	TRP	D	657	117.944	2.158	46.996	1.00	27.78	D
	ATOM	8561	CA	TRP	D	657	117.299	3.256	47.715	1.00	28.29	D
	ATOM	8562	CB	TRP	D	657	118.296	3.913	48.699	1.00	26.47	D
	ATOM	8563	CG	TRP	D	657	119.251	2.947	49.419	1.00	24.99	D
35	ATOM	8564	CD2	TRP	D	657	119.136	2.448	50.768	1.00	23.38	D
	ATOM	8565	CE2	TRP	D	657	120.215	1.554	50.972	1.00	22.65	D
	ATOM	8566	CE3	TRP	D	657	118.226	2.664	51.818	1.00	22.66	D
	ATOM	8567	CD1	TRP	D	657	120.369	2.352	48.891	1.00	22.06	D
	ATOM	8568	NE1	TRP	D	657	120.947	1.520	49.815	1.00	21.92	D
40	ATOM	8569	CZ2	TRP	D	657	120.407	0.875	52.180	1.00	20.78	D
	ATOM	8570	CZ3	TRP	D	657	118.423	1.979	53.026	1.00	22.09	D
	ATOM	8571	CH2	TRP	D	657	119.505	1.098	53.187	1.00	22.26	D
	ATOM	8572	C	TRP	D	657	116.777	4.313	46.705	1.00	29.51	D
	ATOM	8573	O	TRP	D	657	117.304	4.422	45.592	1.00	29.88	D
45	ATOM	8574	N	ASP	D	658	115.744	5.076	47.075	1.00	29.21	D
	ATOM	8575	CA	ASP	D	658	115.223	6.104	46.174	1.00	29.96	D
	ATOM	8576	CB	ASP	D	658	113.977	6.790	46.757	1.00	28.48	D
	ATOM	8577	CG	ASP	D	658	113.460	7.923	45.868	1.00	28.43	D
	ATOM	8578	OD1	ASP	D	658	112.888	7.650	44.793	1.00	28.91	D
50	ATOM	8579	OD2	ASP	D	658	113.628	9.101	46.236	1.00	27.59	D
	ATOM	8580	C	ASP	D	658	116.354	7.113	46.026	1.00	31.50	D
	ATOM	8581	O	ASP	D	658	116.978	7.503	47.017	1.00	32.96	D
	ATOM	8582	N	ALA	D	659	116.621	7.526	44.791	1.00	31.88	D
	ATOM	8583	CA	ALA	D	659	117.694	8.468	44.499	1.00	32.44	D

	ATOM	8584	CB	ALA	D	659	117.811	8.649	43.010	1.00	32.07	D
	ATOM	8585	C	ALA	D	659	117.541	9.829	45.162	1.00	33.56	D
	ATOM	8586	O	ALA	D	659	118.463	10.634	45.141	1.00	34.05	D
	ATOM	8587	N	ASN	D	660	116.387	10.091	45.761	1.00	36.44	D
5	ATOM	8588	CA	ASN	D	660	116.155	11.379	46.400	1.00	37.59	D
	ATOM	8589	CB	ASN	D	660	115.061	12.130	45.645	1.00	39.91	D
	ATOM	8590	CG	ASN	D	660	114.872	13.542	46.149	1.00	43.39	D
	ATOM	8591	OD1	ASN	D	660	114.382	13.764	47.264	1.00	44.43	D
	ATOM	8592	ND2	ASN	D	660	115.274	14.515	45.334	1.00	45.95	D
10	ATOM	8593	C	ASN	D	660	115.791	11.248	47.876	1.00	36.76	D
	ATOM	8594	O	ASN	D	660	116.233	12.050	48.689	1.00	38.43	D
	ATOM	8595	N	ASP	D	661	114.991	10.239	48.214	1.00	35.26	D
	ATOM	8596	CA	ASP	D	661	114.566	9.984	49.592	1.00	33.16	D
	ATOM	8597	CB	ASP	D	661	113.165	9.393	49.620	1.00	34.45	D
15	ATOM	8598	CG	ASP	D	661	112.144	10.331	49.104	1.00	38.11	D
	ATOM	8599	OD1	ASP	D	661	112.280	11.540	49.419	1.00	40.95	D
	ATOM	8600	OD2	ASP	D	661	111.200	9.876	48.409	1.00	39.95	D
	ATOM	8601	C	ASP	D	661	115.458	8.980	50.292	1.00	31.13	D
	ATOM	8602	O	ASP	D	661	115.569	9.004	51.505	1.00	31.79	D
20	ATOM	8603	N	TYR	D	662	116.023	8.062	49.517	1.00	26.92	D
	ATOM	8604	CA	TYR	D	662	116.885	7.016	50.027	1.00	25.03	D
	ATOM	8605	CB	TYR	D	662	118.028	7.615	50.876	1.00	23.52	D
	ATOM	8606	CG	TYR	D	662	118.839	8.622	50.075	1.00	24.99	D
	ATOM	8607	CD1	TYR	D	662	119.614	8.201	48.999	1.00	23.45	D
25	ATOM	8608	CE1	TYR	D	662	120.257	9.099	48.181	1.00	23.80	D
	ATOM	8609	CD2	TYR	D	662	118.739	9.996	50.317	1.00	23.15	D
	ATOM	8610	CE2	TYR	D	662	119.384	10.914	49.497	1.00	24.08	D
	ATOM	8611	CZ	TYR	D	662	120.143	10.459	48.424	1.00	25.80	D
	ATOM	8612	OH	TYR	D	662	120.770	11.367	47.581	1.00	25.60	D
30	ATOM	8613	C	TYR	D	662	116.090	5.979	50.808	1.00	24.80	D
	ATOM	8614	O	TYR	D	662	116.663	5.210	51.590	1.00	25.89	D
	ATOM	8615	N	SER	D	663	114.777	5.946	50.575	1.00	21.66	D
	ATOM	8616	CA	SER	D	663	113.886	4.981	51.228	1.00	21.07	D
	ATOM	8617	CB	SER	D	663	112.432	5.460	51.165	1.00	20.52	D
35	ATOM	8618	OG	SER	D	663	111.987	5.642	49.838	1.00	19.13	D
	ATOM	8619	C	SER	D	663	113.996	3.610	50.564	1.00	20.63	D
	ATOM	8620	O	SER	D	663	114.182	3.530	49.357	1.00	20.77	D
	ATOM	8621	N	ARG	D	664	113.901	2.537	51.353	1.00	21.12	D
	ATOM	8622	CA	ARG	D	664	114.022	1.180	50.819	1.00	20.22	D
40	ATOM	8623	CB	ARG	D	664	113.564	0.125	51.849	1.00	22.66	D
	ATOM	8624	CG	ARG	D	664	114.575	-0.302	52.980	1.00	25.13	D
	ATOM	8625	CD	ARG	D	664	114.860	0.821	53.987	1.00	27.71	D
	ATOM	8626	NE	ARG	D	664	115.573	0.440	55.219	1.00	29.68	D
	ATOM	8627	CZ	ARG	D	664	116.626	-0.373	55.291	1.00	31.69	D
45	ATOM	8628	NH1	ARG	D	664	117.114	-0.935	54.200	1.00	34.72	D
	ATOM	8629	NH2	ARG	D	664	117.226	-0.597	56.456	1.00	30.46	D
	ATOM	8630	C	ARG	D	664	113.196	1.037	49.552	1.00	18.91	D
	ATOM	8631	O	ARG	D	664	112.013	1.393	49.525	1.00	19.59	D
	ATOM	8632	N	LYS	D	665	113.833	0.544	48.496	1.00	17.43	D
50	ATOM	8633	CA	LYS	D	665	113.144	0.320	47.238	1.00	16.40	D
	ATOM	8634	CB	LYS	D	665	113.729	1.204	46.148	1.00	14.06	D
	ATOM	8635	CG	LYS	D	665	113.132	2.582	46.190	1.00	13.78	D
	ATOM	8636	CD	LYS	D	665	111.661	2.434	45.960	1.00	14.84	D
	ATOM	8637	CE	LYS	D	665	110.875	3.713	46.115	1.00	14.42	D

	ATOM	8638	NZ	LYS	D	665	109.447	3.311	45.873	1.00	17.38	D
	ATOM	8639	C	LYS	D	665	113.202	-1.149	46.868	1.00	15.50	D
	ATOM	8640	O	LYS	D	665	112.216	-1.709	46.413	1.00	18.21	D
	ATOM	8641	N	PHE	D	666	114.352	-1.778	47.069	1.00	15.94	D
5	ATOM	8642	CA	PHE	D	666	114.492	-3.207	46.810	1.00	16.38	D
	ATOM	8643	CB	PHE	D	666	114.453	-3.531	45.291	1.00	12.81	D
	ATOM	8644	CG	PHE	D	666	115.613	-2.980	44.477	1.00	13.72	D
	ATOM	8645	CD1	PHE	D	666	116.914	-3.428	44.676	1.00	14.32	D
	ATOM	8646	CD2	PHE	D	666	115.386	-2.051	43.460	1.00	16.32	D
10	ATOM	8647	CE1	PHE	D	666	117.963	-2.962	43.881	1.00	12.43	D
	ATOM	8648	CE2	PHE	D	666	116.433	-1.579	42.659	1.00	14.70	D
	ATOM	8649	CZ	PHE	D	666	117.716	-2.039	42.873	1.00	15.14	D
	ATOM	8650	C	PHE	D	666	115.764	-3.767	47.482	1.00	17.88	D
	ATOM	8651	O	PHE	D	666	116.618	-3.017	47.971	1.00	18.62	D
15	ATOM	8652	N	SER	D	667	115.869	-5.088	47.533	1.00	19.07	D
	ATOM	8653	CA	SER	D	667	117.021	-5.736	48.127	1.00	20.16	D
	ATOM	8654	CB	SER	D	667	116.971	-5.646	49.661	1.00	21.18	D
	ATOM	8655	OG	SER	D	667	115.778	-6.192	50.188	1.00	21.36	D
	ATOM	8656	C	SER	D	667	117.089	-7.188	47.675	1.00	19.78	D
20	ATOM	8657	O	SER	D	667	116.093	-7.907	47.662	1.00	18.38	D
	ATOM	8658	N	TYR	D	668	118.280	-7.596	47.274	1.00	20.33	D
	ATOM	8659	CA	TYR	D	668	118.499	-8.946	46.807	1.00	21.29	D
	ATOM	8660	CB	TYR	D	668	118.756	-8.936	45.293	1.00	21.18	D
	ATOM	8661	CG	TYR	D	668	117.595	-8.369	44.470	1.00	20.55	D
25	ATOM	8662	CD1	TYR	D	668	116.495	-9.171	44.114	1.00	18.14	D
	ATOM	8663	CE1	TYR	D	668	115.423	-8.647	43.403	1.00	18.24	D
	ATOM	8664	CD2	TYR	D	668	117.584	-7.020	44.084	1.00	18.54	D
	ATOM	8665	CE2	TYR	D	668	116.522	-6.484	43.379	1.00	18.25	D
	ATOM	8666	CZ	TYR	D	668	115.437	-7.293	43.044	1.00	19.79	D
30	ATOM	8667	OH	TYR	D	668	114.343	-6.732	42.410	1.00	18.58	D
	ATOM	8668	C	TYR	D	668	119.709	-9.445	47.560	1.00	21.68	D
	ATOM	8669	O	TYR	D	668	120.525	-8.650	48.008	1.00	24.28	D
	ATOM	8670	N	HIS	D	669	119.802	-10.757	47.718	1.00	23.30	D
	ATOM	8671	CA	HIS	D	669	120.904	-11.398	48.413	1.00	23.12	D
35	ATOM	8672	CB	HIS	D	669	120.433	-11.895	49.771	1.00	23.33	D
	ATOM	8673	CG	HIS	D	669	121.343	-11.528	50.897	1.00	26.89	D
	ATOM	8674	CD2	HIS	D	669	121.187	-10.654	51.921	1.00	25.28	D
	ATOM	8675	ND1	HIS	D	669	122.608	-12.060	51.034	1.00	26.65	D
	ATOM	8676	CE1	HIS	D	669	123.193	-11.529	52.093	1.00	27.24	D
40	ATOM	8677	NE2	HIS	D	669	122.353	-10.673	52.649	1.00	27.53	D
	ATOM	8678	C	HIS	D	669	121.274	-12.587	47.535	1.00	24.51	D
	ATOM	8679	O	HIS	D	669	120.399	-13.313	47.036	1.00	24.95	D
	ATOM	8680	N	HIS	D	670	122.569	-12.779	47.335	1.00	24.99	D
	ATOM	8681	CA	HIS	D	670	123.045	-13.882	46.521	1.00	25.59	D
45	ATOM	8682	CB	HIS	D	670	124.501	-13.642	46.121	1.00	26.37	D
	ATOM	8683	CG	HIS	D	670	124.666	-12.905	44.823	1.00	29.01	D
	ATOM	8684	CD2	HIS	D	670	125.637	-12.971	43.881	1.00	27.78	D
	ATOM	8685	ND1	HIS	D	670	123.779	-11.942	44.387	1.00	28.88	D
	ATOM	8686	CE1	HIS	D	670	124.199	-11.450	43.236	1.00	26.47	D
50	ATOM	8687	NE2	HIS	D	670	125.324	-12.055	42.907	1.00	25.99	D
	ATOM	8688	C	HIS	D	670	122.918	-15.176	47.326	1.00	27.14	D
	ATOM	8689	O	HIS	D	670	123.583	-15.346	48.362	1.00	25.08	D
	ATOM	8690	N	THR	D	671	122.059	-16.080	46.840	1.00	28.13	D
	ATOM	8691	CA	THR	D	671	121.796	-17.381	47.473	1.00	27.79	D

5	ATOM	8692	CB	THR	D	671	121.180	-18.369	46.454	1.00	26.12	D
	ATOM	8693	OG1	THR	D	671	119.789	-18.069	46.289	1.00	23.95	D
	ATOM	8694	CG2	THR	D	671	121.312	-19.791	46.930	1.00	26.83	D
	ATOM	8695	C	THR	D	671	122.992	-18.034	48.162	1.00	29.31	D
	ATOM	8696	O	THR	D	671	122.854	-18.547	49.271	1.00	29.25	D
	ATOM	8697	N	ASN	D	672	124.156	-18.025	47.516	1.00	31.23	D
	ATOM	8698	CA	ASN	D	672	125.354	-18.627	48.116	1.00	33.42	D
	ATOM	8699	CB	ASN	D	672	126.498	-18.738	47.089	1.00	35.89	D
10	ATOM	8700	CG	ASN	D	672	126.323	-19.911	46.105	1.00	40.95	D
	ATOM	8701	OD1	ASN	D	672	125.241	-20.116	45.535	1.00	42.75	D
	ATOM	8702	ND2	ASN	D	672	127.406	-20.672	45.887	1.00	42.55	D
	ATOM	8703	C	ASN	D	672	125.861	-17.813	49.317	1.00	33.48	D
15	ATOM	8704	O	ASN	D	672	126.666	-18.302	50.105	1.00	35.72	D
	ATOM	8705	N	LEU	D	673	125.405	-16.574	49.455	1.00	31.40	D
	ATOM	8706	CA	LEU	D	673	125.864	-15.722	50.549	1.00	30.75	D
	ATOM	8707	CB	LEU	D	673	125.631	-16.410	51.901	1.00	30.83	D
	ATOM	8708	CG	LEU	D	673	124.165	-16.514	52.344	1.00	31.99	D
	ATOM	8709	CD1	LEU	D	673	124.059	-17.284	53.649	1.00	32.25	D
20	ATOM	8710	CD2	LEU	D	673	123.580	-15.115	52.510	1.00	33.43	D
	ATOM	8711	C	LEU	D	673	127.346	-15.337	50.420	1.00	28.49	D
	ATOM	8712	O	LEU	D	673	128.045	-15.214	51.429	1.00	29.31	D
	ATOM	8713	N	SER	D	674	127.812	-15.145	49.185	1.00	24.89	D
25	ATOM	8714	CA	SER	D	674	129.201	-14.771	48.911	1.00	23.72	D
	ATOM	8715	CB	SER	D	674	129.764	-15.608	47.764	1.00	23.54	D
	ATOM	8716	OG	SER	D	674	128.969	-15.454	46.598	1.00	27.66	D
	ATOM	8717	C	SER	D	674	129.289	-13.287	48.546	1.00	22.55	D
	ATOM	8718	O	SER	D	674	128.336	-12.721	48.035	1.00	22.93	D
	ATOM	8719	N	ALA	D	675	130.431	-12.657	48.796	1.00	21.17	D
30	ATOM	8720	CA	ALA	D	675	130.580	-11.240	48.498	1.00	20.35	D
	ATOM	8721	CB	ALA	D	675	132.002	-10.779	48.814	1.00	16.29	D
	ATOM	8722	C	ALA	D	675	130.215	-10.836	47.075	1.00	20.97	D
	ATOM	8723	O	ALA	D	675	130.528	-11.527	46.095	1.00	22.46	D
	ATOM	8724	N	ILE	D	676	129.538	-9.703	46.972	1.00	21.38	D
35	ATOM	8725	CA	ILE	D	676	129.180	-9.194	45.667	1.00	23.44	D
	ATOM	8726	CB	ILE	D	676	128.051	-8.132	45.734	1.00	24.56	D
	ATOM	8727	CG2	ILE	D	676	127.897	-7.484	44.377	1.00	23.13	D
	ATOM	8728	CG1	ILE	D	676	126.727	-8.776	46.197	1.00	25.69	D
40	ATOM	8729	CD1	ILE	D	676	126.316	-10.018	45.386	1.00	25.28	D
	ATOM	8730	C	ILE	D	676	130.470	-8.526	45.202	1.00	23.09	D
	ATOM	8731	O	ILE	D	676	130.971	-7.613	45.853	1.00	23.97	D
	ATOM	8732	N	THR	D	677	131.012	-9.000	44.091	1.00	21.72	D
	ATOM	8733	CA	THR	D	677	132.250	-8.474	43.554	1.00	21.86	D
45	ATOM	8734	CB	THR	D	677	133.096	-9.589	42.896	1.00	25.37	D
	ATOM	8735	OG1	THR	D	677	133.515	-10.542	43.884	1.00	25.75	D
	ATOM	8736	CG2	THR	D	677	134.328	-8.977	42.219	1.00	27.86	D
	ATOM	8737	C	THR	D	677	132.001	-7.420	42.488	1.00	20.83	D
	ATOM	8738	O	THR	D	677	132.880	-6.605	42.208	1.00	17.53	D
50	ATOM	8739	N	THR	D	678	130.818	-7.457	41.876	1.00	20.52	D
	ATOM	8740	CA	THR	D	678	130.492	-6.512	40.821	1.00	19.25	D
	ATOM	8741	CB	THR	D	678	131.294	-6.864	39.512	1.00	20.24	D
	ATOM	8742	OG1	THR	D	678	131.093	-5.842	38.533	1.00	19.49	D
	ATOM	8743	CG2	THR	D	678	130.834	-8.193	38.927	1.00	17.27	D
	ATOM	8744	C	THR	D	678	129.001	-6.490	40.495	1.00	18.40	D
	ATOM	8745	O	THR	D	678	128.308	-7.497	40.627	1.00	17.73	D

	ATOM	8746	N	PHE	D	679	128.521	-5.336	40.044	1.00	19.50	D
	ATOM	8747	CA	PHE	D	679	127.119	-5.179	39.653	1.00	20.10	D
	ATOM	8748	CB	PHE	D	679	126.212	-5.151	40.896	1.00	19.62	D
	ATOM	8749	CG	PHE	D	679	126.072	-3.794	41.546	1.00	20.58	D
5	ATOM	8750	CD1	PHE	D	679	125.187	-2.838	41.036	1.00	19.81	D
	ATOM	8751	CD2	PHE	D	679	126.786	-3.493	42.708	1.00	22.11	D
	ATOM	8752	CE1	PHE	D	679	125.008	-1.595	41.679	1.00	19.56	D
	ATOM	8753	CE2	PHE	D	679	126.622	-2.255	43.369	1.00	21.42	D
	ATOM	8754	CZ	PHE	D	679	125.730	-1.305	42.855	1.00	20.49	D
10	ATOM	8755	C	PHE	D	679	126.967	-3.908	38.836	1.00	18.56	D
	ATOM	8756	O	PHE	D	679	127.824	-3.040	38.902	1.00	18.64	D
	ATOM	8757	N	TYR	D	680	125.900	-3.826	38.038	1.00	18.73	D
	ATOM	8758	CA	TYR	D	680	125.610	-2.640	37.216	1.00	18.62	D
	ATOM	8759	CB	TYR	D	680	126.140	-2.818	35.776	1.00	19.64	D
15	ATOM	8760	CG	TYR	D	680	126.416	-1.498	35.070	1.00	21.94	D
	ATOM	8761	CD1	TYR	D	680	127.503	-0.704	35.447	1.00	21.42	D
	ATOM	8762	CE1	TYR	D	680	127.691	0.578	34.917	1.00	21.58	D
	ATOM	8763	CD2	TYR	D	680	125.525	-0.982	34.123	1.00	21.80	D
	ATOM	8764	CE2	TYR	D	680	125.702	0.304	33.585	1.00	21.45	D
20	ATOM	8765	CZ	TYR	D	680	126.780	1.083	33.992	1.00	21.61	D
	ATOM	8766	OH	TYR	D	680	126.891	2.384	33.541	1.00	21.38	D
	ATOM	8767	C	TYR	D	680	124.087	-2.429	37.194	1.00	18.89	D
	ATOM	8768	O	TYR	D	680	123.326	-3.394	37.244	1.00	21.29	D
	ATOM	8769	N	VAL	D	681	123.635	-1.182	37.148	1.00	18.55	D
25	ATOM	8770	CA	VAL	D	681	122.202	-0.952	37.112	1.00	20.06	D
	ATOM	8771	CB	VAL	D	681	121.588	-0.612	38.502	1.00	19.46	D
	ATOM	8772	CG1	VAL	D	681	121.748	-1.770	39.427	1.00	23.82	D
	ATOM	8773	CG2	VAL	D	681	122.219	0.634	39.080	1.00	18.66	D
	ATOM	8774	C	VAL	D	681	121.699	0.134	36.196	1.00	21.12	D
30	ATOM	8775	O	VAL	D	681	122.429	1.030	35.748	1.00	19.50	D
	ATOM	8776	N	SER	D	682	120.404	0.039	35.956	1.00	22.21	D
	ATOM	8777	CA	SER	D	682	119.698	0.991	35.147	1.00	21.87	D
	ATOM	8778	CB	SER	D	682	119.633	0.520	33.703	1.00	20.44	D
	ATOM	8779	OG	SER	D	682	118.589	-0.410	33.525	1.00	21.95	D
35	ATOM	8780	C	SER	D	682	118.331	0.950	35.783	1.00	23.11	D
	ATOM	8781	O	SER	D	682	118.048	0.053	36.582	1.00	22.65	D
	ATOM	8782	N	ASP	D	683	117.483	1.910	35.457	1.00	23.07	D
	ATOM	8783	CA	ASP	D	683	116.165	1.901	36.050	1.00	23.72	D
	ATOM	8784	CB	ASP	D	683	115.359	3.107	35.591	1.00	26.85	D
40	ATOM	8785	CG	ASP	D	683	115.822	4.384	36.224	1.00	30.20	D
	ATOM	8786	OD1	ASP	D	683	116.151	4.341	37.431	1.00	35.54	D
	ATOM	8787	OD2	ASP	D	683	115.840	5.421	35.521	1.00	28.97	D
	ATOM	8788	C	ASP	D	683	115.381	0.631	35.728	1.00	22.90	D
	ATOM	8789	O	ASP	D	683	114.466	0.281	36.458	1.00	22.58	D
45	ATOM	8790	N	ASN	D	684	115.717	-0.072	34.653	1.00	21.68	D
	ATOM	8791	CA	ASN	D	684	114.937	-1.257	34.335	1.00	21.96	D
	ATOM	8792	CB	ASN	D	684	114.568	-1.291	32.842	1.00	20.91	D
	ATOM	8793	CG	ASN	D	684	113.639	-0.138	32.417	1.00	22.88	D
	ATOM	8794	OD1	ASN	D	684	112.685	0.229	33.132	1.00	20.08	D
50	ATOM	8795	ND2	ASN	D	684	113.907	0.423	31.231	1.00	21.27	D
	ATOM	8796	C	ASN	D	684	115.561	-2.597	34.705	1.00	22.28	D
	ATOM	8797	O	ASN	D	684	114.840	-3.557	34.983	1.00	21.62	D
	ATOM	8798	N	ILE	D	685	116.890	-2.659	34.735	1.00	22.22	D
	ATOM	8799	CA	ILE	D	685	117.592	-3.906	35.022	1.00	24.26	D

5	ATOM	8800	CB	ILE	D	685	118.241	-4.431	33.725	1.00	25.72	D
	ATOM	8801	CG2	ILE	D	685	119.014	-5.722	33.987	1.00	28.28	D
	ATOM	8802	CG1	ILE	D	685	117.181	-4.607	32.646	1.00	26.62	D
	ATOM	8803	CD1	ILE	D	685	117.527	-3.851	31.344	1.00	32.32	D
	ATOM	8804	C	ILE	D	685	118.701	-3.830	36.081	1.00	25.44	D
	ATOM	8805	O	ILE	D	685	119.291	-2.771	36.300	1.00	25.75	D
	ATOM	8806	N	LEU	D	686	118.989	-4.964	36.717	1.00	25.66	D
10	ATOM	8807	CA	LEU	D	686	120.069	-5.041	37.689	1.00	26.90	D
	ATOM	8808	CB	LEU	D	686	119.530	-5.089	39.127	1.00	26.08	D
	ATOM	8809	CG	LEU	D	686	120.472	-5.572	40.262	1.00	23.99	D
	ATOM	8810	CD1	LEU	D	686	121.709	-4.699	40.345	1.00	23.40	D
	ATOM	8811	CD2	LEU	D	686	119.740	-5.567	41.585	1.00	21.28	D
15	ATOM	8812	C	LEU	D	686	120.859	-6.317	37.412	1.00	28.01	D
	ATOM	8813	O	LEU	D	686	120.275	-7.397	37.340	1.00	28.42	D
	ATOM	8814	N	VAL	D	687	122.170	-6.194	37.226	1.00	26.81	D
	ATOM	8815	CA	VAL	D	687	122.995	-7.371	37.019	1.00	28.16	D
	ATOM	8816	CB	VAL	D	687	123.648	-7.401	35.629	1.00	28.88	D
	ATOM	8817	CG1	VAL	D	687	124.496	-8.669	35.484	1.00	27.76	D
	ATOM	8818	CG2	VAL	D	687	122.562	-7.383	34.553	1.00	29.55	D
20	ATOM	8819	C	VAL	D	687	124.064	-7.347	38.098	1.00	29.32	D
	ATOM	8820	O	VAL	D	687	124.744	-6.331	38.291	1.00	29.09	D
	ATOM	8821	N	SER	D	688	124.200	-8.465	38.813	1.00	28.34	D
	ATOM	8822	CA	SER	D	688	125.166	-8.570	39.910	1.00	27.42	D
	ATOM	8823	CB	SER	D	688	124.419	-8.567	41.247	1.00	26.52	D
25	ATOM	8824	OG	SER	D	688	123.505	-9.651	41.304	1.00	25.52	D
	ATOM	8825	C	SER	D	688	125.990	-9.853	39.808	1.00	27.67	D
	ATOM	8826	O	SER	D	688	125.518	-10.870	39.304	1.00	28.15	D
	ATOM	8827	N	GLY	D	689	127.217	-9.818	40.299	1.00	25.88	D
	ATOM	8828	CA	GLY	D	689	128.012	-11.016	40.228	1.00	25.97	D
30	ATOM	8829	C	GLY	D	689	128.901	-11.218	41.422	1.00	27.10	D
	ATOM	8830	O	GLY	D	689	129.549	-10.285	41.890	1.00	29.72	D
	ATOM	8831	N	SER	D	690	128.914	-12.445	41.922	1.00	27.15	D
	ATOM	8832	CA	SER	D	690	129.752	-12.819	43.042	1.00	27.45	D
	ATOM	8833	CB	SER	D	690	128.918	-13.015	44.300	1.00	26.48	D
35	ATOM	8834	OG	SER	D	690	127.975	-14.044	44.099	1.00	25.71	D
	ATOM	8835	C	SER	D	690	130.376	-14.145	42.630	1.00	28.76	D
	ATOM	8836	O	SER	D	690	130.435	-14.457	41.444	1.00	28.74	D
	ATOM	8837	N	GLU	D	691	130.829	-14.925	43.609	1.00	29.69	D
	ATOM	8838	CA	GLU	D	691	131.446	-16.210	43.320	1.00	29.80	D
40	ATOM	8839	CB	GLU	D	691	132.241	-16.711	44.532	1.00	30.89	D
	ATOM	8840	CG	GLU	D	691	132.740	-18.153	44.426	1.00	34.76	D
	ATOM	8841	CD	GLU	D	691	133.806	-18.516	45.469	1.00	37.18	D
	ATOM	8842	OE1	GLU	D	691	134.895	-17.901	45.448	1.00	39.22	D
	ATOM	8843	OE2	GLU	D	691	133.564	-19.420	46.305	1.00	38.14	D
45	ATOM	8844	C	GLU	D	691	130.409	-17.239	42.888	1.00	29.94	D
	ATOM	8845	O	GLU	D	691	129.441	-17.507	43.596	1.00	28.81	D
	ATOM	8846	N	ASN	D	692	130.621	-17.784	41.693	1.00	30.68	D
	ATOM	8847	CA	ASN	D	692	129.756	-18.800	41.122	1.00	30.63	D
	ATOM	8848	CB	ASN	D	692	129.854	-20.070	41.975	1.00	32.82	D
50	ATOM	8849	CG	ASN	D	692	131.019	-20.951	41.562	1.00	34.81	D
	ATOM	8850	OD1	ASN	D	692	130.832	-21.908	40.812	1.00	39.00	D
	ATOM	8851	ND2	ASN	D	692	132.231	-20.614	42.016	1.00	34.40	D
	ATOM	8852	C	ASN	D	692	128.313	-18.370	40.941	1.00	30.73	D
	ATOM	8853	O	ASN	D	692	127.395	-19.187	40.996	1.00	31.82	D

	ATOM	8854	N	GLN	D	693	128.113	-17.081	40.711	1.00	30.83	D
	ATOM	8855	CA	GLN	D	693	126.774	-16.564	40.496	1.00	30.85	D
	ATOM	8856	CB	GLN	D	693	126.127	-16.215	41.837	1.00	32.95	D
	ATOM	8857	CG	GLN	D	693	125.494	-17.398	42.562	1.00	36.48	D
5	ATOM	8858	CD	GLN	D	693	124.636	-16.949	43.741	1.00	39.48	D
	ATOM	8859	OE1	GLN	D	693	123.650	-16.222	43.571	1.00	40.51	D
	ATOM	8860	NE2	GLN	D	693	125.014	-17.371	44.941	1.00	40.67	D
	ATOM	8861	C	GLN	D	693	126.771	-15.350	39.560	1.00	30.20	D
	ATOM	8862	O	GLN	D	693	127.694	-14.533	39.586	1.00	28.95	D
10	ATOM	8863	N	PHE	D	694	125.729	-15.268	38.728	1.00	28.92	D
	ATOM	8864	CA	PHE	D	694	125.534	-14.189	37.758	1.00	27.46	D
	ATOM	8865	CB	PHE	D	694	126.183	-14.549	36.404	1.00	26.85	D
	ATOM	8866	CG	PHE	D	694	126.212	-13.402	35.413	1.00	27.99	D
	ATOM	8867	CD1	PHE	D	694	127.027	-12.290	35.626	1.00	28.31	D
15	ATOM	8868	CD2	PHE	D	694	125.387	-13.411	34.291	1.00	28.25	D
	ATOM	8869	CE1	PHE	D	694	127.011	-11.201	34.734	1.00	25.87	D
	ATOM	8870	CE2	PHE	D	694	125.365	-12.329	33.397	1.00	26.35	D
	ATOM	8871	CZ	PHE	D	694	126.175	-11.226	33.620	1.00	24.43	D
	ATOM	8872	C	PHE	D	694	124.018	-14.020	37.600	1.00	26.65	D
20	ATOM	8873	O	PHE	D	694	123.360	-14.804	36.923	1.00	27.90	D
	ATOM	8874	N	ASN	D	695	123.462	-12.997	38.235	1.00	25.11	D
	ATOM	8875	CA	ASN	D	695	122.033	-12.784	38.169	1.00	22.66	D
	ATOM	8876	CB	ASN	D	695	121.462	-12.735	39.570	1.00	21.74	D
	ATOM	8877	CG	ASN	D	695	121.802	-13.948	40.351	1.00	22.53	D
25	ATOM	8878	OD1	ASN	D	695	122.469	-13.863	41.381	1.00	25.44	D
	ATOM	8879	ND2	ASN	D	695	121.369	-15.102	39.866	1.00	21.60	D
	ATOM	8880	C	ASN	D	695	121.586	-11.557	37.431	1.00	22.56	D
	ATOM	8881	O	ASN	D	695	122.283	-10.537	37.402	1.00	24.25	D
	ATOM	8882	N	ILE	D	696	120.407	-11.675	36.828	1.00	20.27	D
30	ATOM	8883	CA	ILE	D	696	119.785	-10.570	36.112	1.00	18.17	D
	ATOM	8884	CB	ILE	D	696	119.741	-10.848	34.598	1.00	13.96	D
	ATOM	8885	CG2	ILE	D	696	119.173	-9.631	33.874	1.00	12.40	D
	ATOM	8886	CG1	ILE	D	696	121.165	-11.096	34.095	1.00	11.96	D
	ATOM	8887	CD1	ILE	D	696	121.278	-11.411	32.627	1.00	10.15	D
35	ATOM	8888	C	ILE	D	696	118.375	-10.387	36.708	1.00	19.43	D
	ATOM	8889	O	ILE	D	696	117.558	-11.307	36.714	1.00	19.49	D
	ATOM	8890	N	TYR	D	697	118.130	-9.194	37.236	1.00	18.77	D
	ATOM	8891	CA	TYR	D	697	116.878	-8.867	37.881	1.00	17.94	D
	ATOM	8892	CB	TYR	D	697	117.167	-8.295	39.280	1.00	19.60	D
40	ATOM	8893	CG	TYR	D	697	118.014	-9.185	40.171	1.00	19.57	D
	ATOM	8894	CD1	TYR	D	697	117.428	-10.186	40.962	1.00	20.99	D
	ATOM	8895	CE1	TYR	D	697	118.204	-11.012	41.789	1.00	18.57	D
	ATOM	8896	CD2	TYR	D	697	119.397	-9.031	40.223	1.00	18.67	D
	ATOM	8897	CE2	TYR	D	697	120.179	-9.840	41.035	1.00	19.21	D
45	ATOM	8898	CZ	TYR	D	697	119.581	-10.832	41.820	1.00	20.43	D
	ATOM	8899	OH	TYR	D	697	120.372	-11.634	42.627	1.00	20.44	D
	ATOM	8900	C	TYR	D	697	116.059	-7.843	37.104	1.00	18.57	D
	ATOM	8901	O	TYR	D	697	116.604	-6.934	36.456	1.00	18.53	D
	ATOM	8902	N	ASN	D	698	114.746	-7.975	37.208	1.00	16.25	D
50	ATOM	8903	CA	ASN	D	698	113.826	-7.049	36.575	1.00	16.13	D
	ATOM	8904	CB	ASN	D	698	112.594	-7.832	36.111	1.00	16.70	D
	ATOM	8905	CG	ASN	D	698	111.516	-6.939	35.508	1.00	18.93	D
	ATOM	8906	OD1	ASN	D	698	111.253	-5.822	36.004	1.00	16.72	D
	ATOM	8907	ND2	ASN	D	698	110.873	-7.428	34.443	1.00	16.48	D

	ATOM	8908	C	ASN	D	698	113.441	-6.032	37.682	1.00	15.83	D
	ATOM	8909	O	ASN	D	698	112.568	-6.301	38.499	1.00	14.84	D
	ATOM	8910	N	LEU	D	699	114.078	-4.874	37.735	1.00	14.22	D
	ATOM	8911	CA	LEU	D	699	113.725	-3.948	38.796	1.00	15.47	D
5	ATOM	8912	CB	LEU	D	699	114.549	-2.673	38.704	1.00	11.67	D
	ATOM	8913	CG	LEU	D	699	115.818	-2.596	39.541	1.00	12.58	D
	ATOM	8914	CD1	LEU	D	699	116.357	-4.000	39.957	1.00	9.17	D
	ATOM	8915	CD2	LEU	D	699	116.822	-1.809	38.724	1.00	9.81	D
	ATOM	8916	C	LEU	D	699	112.260	-3.560	38.883	1.00	18.10	D
10	ATOM	8917	O	LEU	D	699	111.836	-3.053	39.914	1.00	21.11	D
	ATOM	8918	N	ARG	D	700	111.479	-3.765	37.826	1.00	19.06	D
	ATOM	8919	CA	ARG	D	700	110.063	-3.382	37.889	1.00	18.41	D
	ATOM	8920	CB	ARG	D	700	109.474	-3.190	36.481	1.00	16.13	D
	ATOM	8921	CG	ARG	D	700	110.078	-2.053	35.660	1.00	18.32	D
15	ATOM	8922	CD	ARG	D	700	109.605	-2.100	34.188	1.00	19.47	D
	ATOM	8923	NE	ARG	D	700	110.340	-1.195	33.295	1.00	19.60	D
	ATOM	8924	CZ	ARG	D	700	109.881	-0.738	32.127	1.00	20.84	D
	ATOM	8925	NH1	ARG	D	700	108.678	-1.085	31.693	1.00	19.16	D
	ATOM	8926	NH2	ARG	D	700	110.633	0.057	31.378	1.00	20.52	D
20	ATOM	8927	C	ARG	D	700	109.211	-4.411	38.652	1.00	19.19	D
	ATOM	8928	O	ARG	D	700	108.440	-4.069	39.546	1.00	20.01	D
	ATOM	8929	N	SER	D	701	109.344	-5.673	38.286	1.00	18.61	D
	ATOM	8930	CA	SER	D	701	108.580	-6.719	38.919	1.00	18.99	D
	ATOM	8931	CB	SER	D	701	108.403	-7.907	37.960	1.00	17.26	D
25	ATOM	8932	OG	SER	D	701	109.627	-8.299	37.350	1.00	16.41	D
	ATOM	8933	C	SER	D	701	109.317	-7.179	40.154	1.00	21.34	D
	ATOM	8934	O	SER	D	701	108.758	-7.881	40.983	1.00	21.67	D
	ATOM	8935	N	GLY	D	702	110.577	-6.782	40.277	1.00	23.17	D
	ATOM	8936	CA	GLY	D	702	111.367	-7.189	41.420	1.00	25.46	D
30	ATOM	8937	C	GLY	D	702	111.916	-8.601	41.338	1.00	26.82	D
	ATOM	8938	O	GLY	D	702	112.676	-9.008	42.208	1.00	28.70	D
	ATOM	8939	N	LYS	D	703	111.580	-9.346	40.290	1.00	28.39	D
	ATOM	8940	CA	LYS	D	703	112.040	-10.734	40.187	1.00	29.97	D
	ATOM	8941	CB	LYS	D	703	110.926	-11.616	39.609	1.00	30.86	D
35	ATOM	8942	CG	LYS	D	703	109.566	-11.294	40.211	1.00	34.24	D
	ATOM	8943	CD	LYS	D	703	108.553	-12.393	40.031	1.00	36.04	D
	ATOM	8944	CE	LYS	D	703	108.971	-13.657	40.786	1.00	38.38	D
	ATOM	8945	NZ	LYS	D	703	107.900	-14.711	40.780	1.00	39.62	D
	ATOM	8946	C	LYS	D	703	113.319	-11.022	39.428	1.00	30.16	D
40	ATOM	8947	O	LYS	D	703	113.822	-10.202	38.665	1.00	33.16	D
	ATOM	8948	N	LEU	D	704	113.824	-12.227	39.655	1.00	31.22	D
	ATOM	8949	CA	LEU	D	704	115.037	-12.717	39.024	1.00	31.13	D
	ATOM	8950	CB	LEU	D	704	115.655	-13.799	39.894	1.00	28.59	D
	ATOM	8951	CG	LEU	D	704	116.959	-14.425	39.433	1.00	29.39	D
45	ATOM	8952	CD1	LEU	D	704	118.092	-13.385	39.446	1.00	31.25	D
	ATOM	8953	CD2	LEU	D	704	117.298	-15.548	40.368	1.00	27.62	D
	ATOM	8954	C	LEU	D	704	114.663	-13.302	37.668	1.00	32.42	D
	ATOM	8955	O	LEU	D	704	113.791	-14.167	37.585	1.00	34.11	D
	ATOM	8956	N	VAL	D	705	115.308	-12.827	36.607	1.00	32.96	D
50	ATOM	8957	CA	VAL	D	705	115.014	-13.329	35.275	1.00	33.27	D
	ATOM	8958	CB	VAL	D	705	115.052	-12.240	34.214	1.00	31.84	D
	ATOM	8959	CG1	VAL	D	705	114.710	-12.853	32.866	1.00	33.49	D
	ATOM	8960	CG2	VAL	D	705	114.079	-11.142	34.544	1.00	30.65	D
	ATOM	8961	C	VAL	D	705	116.011	-14.389	34.841	1.00	35.05	D

	ATOM	8962	O	VAL	D	705	115.632	-15.501	34.504	1.00	37.11	D
	ATOM	8963	N	HIS	D	706	117.291	-14.041	34.827	1.00	36.45	D
	ATOM	8964	CA	HIS	D	706	118.316	-14.991	34.426	1.00	36.74	D
	ATOM	8965	CB	HIS	D	706	119.007	-14.539	33.137	1.00	37.71	D
5	ATOM	8966	CG	HIS	D	706	118.064	-14.142	32.042	1.00	40.20	D
	ATOM	8967	CD2	HIS	D	706	117.901	-12.964	31.392	1.00	41.01	D
	ATOM	8968	ND1	HIS	D	706	117.172	-15.022	31.468	1.00	40.45	D
	ATOM	8969	CE1	HIS	D	706	116.504	-14.404	30.509	1.00	41.40	D
	ATOM	8970	NE2	HIS	D	706	116.927	-13.155	30.441	1.00	41.00	D
10	ATOM	8971	C	HIS	D	706	119.361	-15.155	35.527	1.00	37.89	D
	ATOM	8972	O	HIS	D	706	119.869	-14.174	36.096	1.00	38.65	D
	ATOM	8973	N	ALA	D	707	119.686	-16.414	35.805	1.00	37.80	D
	ATOM	8974	CA	ALA	D	707	120.660	-16.757	36.828	1.00	36.66	D
	ATOM	8975	CB	ALA	D	707	119.935	-17.223	38.075	1.00	33.53	D
15	ATOM	8976	C	ALA	D	707	121.651	-17.828	36.367	1.00	36.44	D
	ATOM	8977	O	ALA	D	707	122.608	-18.138	37.079	1.00	36.66	D
	ATOM	8978	N	ASN	D	708	121.446	-18.382	35.177	1.00	36.37	D
	ATOM	8979	CA	ASN	D	708	122.347	-19.431	34.710	1.00	37.18	D
	ATOM	8980	CB	ASN	D	708	121.553	-20.739	34.521	1.00	37.73	D
20	ATOM	8981	CG	ASN	D	708	120.893	-21.212	35.821	1.00	38.57	D
	ATOM	8982	OD1	ASN	D	708	119.667	-21.227	35.947	1.00	38.35	D
	ATOM	8983	ND2	ASN	D	708	121.712	-21.588	36.794	1.00	37.37	D
	ATOM	8984	C	ASN	D	708	123.137	-19.084	33.443	1.00	36.59	D
	ATOM	8985	O	ASN	D	708	123.856	-19.927	32.907	1.00	35.29	D
25	ATOM	8986	N	ILE	D	709	123.019	-17.839	32.986	1.00	35.82	D
	ATOM	8987	CA	ILE	D	709	123.709	-17.402	31.781	1.00	34.43	D
	ATOM	8988	CB	ILE	D	709	123.349	-15.928	31.408	1.00	32.34	D
	ATOM	8989	CG2	ILE	D	709	124.151	-15.460	30.221	1.00	30.43	D
	ATOM	8990	CG1	ILE	D	709	121.875	-15.836	31.017	1.00	30.65	D
30	ATOM	8991	CD1	ILE	D	709	121.444	-14.459	30.565	1.00	28.79	D
	ATOM	8992	C	ILE	D	709	125.216	-17.552	31.873	1.00	34.88	D
	ATOM	8993	O	ILE	D	709	125.863	-17.878	30.882	1.00	36.86	D
	ATOM	8994	N	LEU	D	710	125.785	-17.336	33.051	1.00	34.63	D
	ATOM	8995	CA	LEU	D	710	127.232	-17.454	33.186	1.00	32.46	D
35	ATOM	8996	CB	LEU	D	710	127.837	-16.058	33.402	1.00	28.39	D
	ATOM	8997	CG	LEU	D	710	128.450	-15.306	32.208	1.00	25.87	D
	ATOM	8998	CD1	LEU	D	710	127.798	-15.707	30.894	1.00	24.33	D
	ATOM	8999	CD2	LEU	D	710	128.331	-13.810	32.443	1.00	23.04	D
	ATOM	9000	C	LEU	D	710	127.683	-18.434	34.269	1.00	33.52	D
40	ATOM	9001	O	LEU	D	710	128.730	-18.246	34.882	1.00	34.43	D
	ATOM	9002	N	LYS	D	711	126.902	-19.494	34.480	1.00	34.36	D
	ATOM	9003	CA	LYS	D	711	127.230	-20.518	35.481	1.00	35.44	D
	ATOM	9004	CB	LYS	D	711	126.238	-21.670	35.389	1.00	34.96	D
	ATOM	9005	CG	LYS	D	711	125.872	-22.006	33.980	1.00	36.79	D
45	ATOM	9006	CD	LYS	D	711	124.620	-22.834	33.940	1.00	38.39	D
	ATOM	9007	CE	LYS	D	711	124.936	-24.285	34.192	1.00	40.21	D
	ATOM	9008	NZ	LYS	D	711	125.841	-24.794	33.104	1.00	42.27	D
	ATOM	9009	C	LYS	D	711	128.645	-21.068	35.350	1.00	36.53	D
	ATOM	9010	O	LYS	D	711	129.284	-21.427	36.341	1.00	36.63	D
50	ATOM	9011	N	ASP	D	712	129.130	-21.126	34.121	1.00	37.64	D
	ATOM	9012	CA	ASP	D	712	130.457	-21.629	33.836	1.00	39.74	D
	ATOM	9013	CB	ASP	D	712	130.688	-21.555	32.336	1.00	44.17	D
	ATOM	9014	CG	ASP	D	712	129.490	-22.032	31.558	1.00	49.91	D
	ATOM	9015	OD1	ASP	D	712	129.338	-23.276	31.408	1.00	53.21	D

	ATOM	9016	OD2	ASP	D	712	128.684	-21.163	31.122	1.00	51.40	D
	ATOM	9017	C	ASP	D	712	131.548	-20.856	34.551	1.00	39.02	D
	ATOM	9018	O	ASP	D	712	132.528	-21.439	34.992	1.00	39.79	D
	ATOM	9019	N	ALA	D	713	131.398	-19.542	34.647	1.00	37.44	D
5	ATOM	9020	CA	ALA	D	713	132.427	-18.740	35.295	1.00	37.31	D
	ATOM	9021	CB	ALA	D	713	132.131	-17.254	35.119	1.00	37.40	D
	ATOM	9022	C	ALA	D	713	132.603	-19.055	36.775	1.00	36.89	D
	ATOM	9023	O	ALA	D	713	131.693	-19.535	37.437	1.00	37.66	D
	ATOM	9024	N	ASP	D	714	133.785	-18.782	37.296	1.00	35.36	D
10	ATOM	9025	CA	ASP	D	714	134.018	-19.033	38.693	1.00	34.87	D
	ATOM	9026	CB	ASP	D	714	135.384	-19.678	38.893	1.00	33.94	D
	ATOM	9027	CG	ASP	D	714	135.484	-21.038	38.244	1.00	32.23	D
	ATOM	9028	OD1	ASP	D	714	134.599	-21.877	38.477	1.00	32.51	D
	ATOM	9029	OD2	ASP	D	714	136.456	-21.279	37.505	1.00	34.54	D
15	ATOM	9030	C	ASP	D	714	133.946	-17.705	39.433	1.00	35.72	D
	ATOM	9031	O	ASP	D	714	133.610	-17.651	40.616	1.00	35.20	D
	ATOM	9032	N	GLN	D	715	134.238	-16.629	38.714	1.00	35.93	D
	ATOM	9033	CA	GLN	D	715	134.233	-15.293	39.284	1.00	36.18	D
	ATOM	9034	CB	GLN	D	715	135.648	-14.938	39.750	1.00	37.10	D
20	ATOM	9035	CG	GLN	D	715	136.260	-15.951	40.716	1.00	39.05	D
	ATOM	9036	CD	GLN	D	715	135.897	-15.672	42.165	1.00	40.12	D
	ATOM	9037	OE1	GLN	D	715	134.751	-15.380	42.472	1.00	42.68	D
	ATOM	9038	NE2	GLN	D	715	136.874	-15.763	43.057	1.00	39.97	D
	ATOM	9039	C	GLN	D	715	133.756	-14.264	38.254	1.00	35.81	D
25	ATOM	9040	O	GLN	D	715	133.993	-14.407	37.054	1.00	35.76	D
	ATOM	9041	N	ILE	D	716	133.073	-13.232	38.736	1.00	34.56	D
	ATOM	9042	CA	ILE	D	716	132.582	-12.149	37.888	1.00	32.51	D
	ATOM	9043	CB	ILE	D	716	131.061	-11.982	38.032	1.00	31.79	D
	ATOM	9044	CG2	ILE	D	716	130.547	-11.006	36.996	1.00	30.49	D
30	ATOM	9045	CG1	ILE	D	716	130.363	-13.336	37.890	1.00	33.24	D
	ATOM	9046	CD1	ILE	D	716	130.638	-14.060	36.579	1.00	34.30	D
	ATOM	9047	C	ILE	D	716	133.285	-10.863	38.375	1.00	32.59	D
	ATOM	9048	O	ILE	D	716	132.797	-10.160	39.264	1.00	33.77	D
	ATOM	9049	N	TRP	D	717	134.444	-10.580	37.795	1.00	30.84	D
35	ATOM	9050	CA	TRP	D	717	135.252	-9.429	38.162	1.00	29.11	D
	ATOM	9051	CB	TRP	D	717	136.558	-9.454	37.379	1.00	32.71	D
	ATOM	9052	CG	TRP	D	717	137.348	-10.687	37.596	1.00	35.43	D
	ATOM	9053	CD2	TRP	D	717	137.669	-11.278	38.855	1.00	35.53	D
	ATOM	9054	CE2	TRP	D	717	138.462	-12.416	38.589	1.00	36.83	D
40	ATOM	9055	CE3	TRP	D	717	137.364	-10.960	40.185	1.00	35.83	D
	ATOM	9056	CD1	TRP	D	717	137.940	-11.464	36.640	1.00	36.35	D
	ATOM	9057	NE1	TRP	D	717	138.612	-12.504	37.230	1.00	37.07	D
	ATOM	9058	CZ2	TRP	D	717	138.956	-13.237	39.605	1.00	38.32	D
	ATOM	9059	CZ3	TRP	D	717	137.855	-11.780	41.193	1.00	37.12	D
45	ATOM	9060	CH2	TRP	D	717	138.641	-12.904	40.896	1.00	37.38	D
	ATOM	9061	C	TRP	D	717	134.583	-8.102	37.930	1.00	26.79	D
	ATOM	9062	O	TRP	D	717	134.507	-7.262	38.825	1.00	24.62	D
	ATOM	9063	N	SER	D	718	134.110	-7.899	36.713	1.00	24.96	D
	ATOM	9064	CA	SER	D	718	133.473	-6.639	36.403	1.00	23.33	D
50	ATOM	9065	CB	SER	D	718	134.499	-5.674	35.830	1.00	21.39	D
	ATOM	9066	OG	SER	D	718	133.898	-4.420	35.620	1.00	24.14	D
	ATOM	9067	C	SER	D	718	132.347	-6.825	35.421	1.00	22.63	D
	ATOM	9068	O	SER	D	718	132.481	-7.549	34.443	1.00	25.60	D
	ATOM	9069	N	VAL	D	719	131.228	-6.175	35.679	1.00	21.31	D

	ATOM	9070	CA	VAL	D	719	130.095	-6.286	34.784	1.00	23.17	D
	ATOM	9071	CB	VAL	D	719	128.900	-6.926	35.517	1.00	23.18	D
	ATOM	9072	CG1	VAL	D	719	128.244	-5.916	36.483	1.00	23.48	D
	ATOM	9073	CG2	VAL	D	719	127.915	-7.427	34.517	1.00	24.77	D
5	ATOM	9074	C	VAL	D	719	129.703	-4.887	34.255	1.00	24.78	D
	ATOM	9075	O	VAL	D	719	130.024	-3.864	34.872	1.00	25.63	D
	ATOM	9076	N	ASN	D	720	129.005	-4.835	33.125	1.00	25.17	D
	ATOM	9077	CA	ASN	D	720	128.604	-3.547	32.543	1.00	25.66	D
	ATOM	9078	CB	ASN	D	720	129.844	-2.787	31.999	1.00	25.58	D
10	ATOM	9079	CG	ASN	D	720	129.627	-1.256	31.853	1.00	26.08	D
	ATOM	9080	OD1	ASN	D	720	128.697	-0.790	31.193	1.00	24.37	D
	ATOM	9081	ND2	ASN	D	720	130.527	-0.484	32.456	1.00	24.14	D
	ATOM	9082	C	ASN	D	720	127.665	-3.882	31.397	1.00	25.69	D
	ATOM	9083	O	ASN	D	720	127.961	-4.770	30.601	1.00	24.75	D
15	ATOM	9084	N	PHE	D	721	126.524	-3.209	31.324	1.00	25.70	D
	ATOM	9085	CA	PHE	D	721	125.610	-3.473	30.226	1.00	25.92	D
	ATOM	9086	CB	PHE	D	721	124.486	-4.426	30.663	1.00	24.85	D
	ATOM	9087	CG	PHE	D	721	123.483	-3.803	31.566	1.00	23.85	D
	ATOM	9088	CD1	PHE	D	721	122.441	-3.052	31.043	1.00	22.92	D
20	ATOM	9089	CD2	PHE	D	721	123.588	-3.938	32.941	1.00	22.57	D
	ATOM	9090	CE1	PHE	D	721	121.525	-2.442	31.877	1.00	21.91	D
	ATOM	9091	CE2	PHE	D	721	122.675	-3.328	33.777	1.00	22.55	D
	ATOM	9092	CZ	PHE	D	721	121.640	-2.579	33.243	1.00	21.48	D
	ATOM	9093	C	PHE	D	721	125.076	-2.145	29.706	1.00	26.21	D
25	ATOM	9094	O	PHE	D	721	125.149	-1.120	30.402	1.00	25.17	D
	ATOM	9095	N	LYS	D	722	124.564	-2.166	28.473	1.00	26.41	D
	ATOM	9096	CA	LYS	D	722	124.046	-0.966	27.801	1.00	25.77	D
	ATOM	9097	CB	LYS	D	722	125.230	-0.140	27.287	1.00	25.66	D
	ATOM	9098	CG	LYS	D	722	125.220	1.340	27.627	1.00	26.55	D
30	ATOM	9099	CD	LYS	D	722	124.193	2.106	26.828	1.00	28.07	D
	ATOM	9100	CE	LYS	D	722	124.609	3.586	26.571	1.00	31.04	D
	ATOM	9101	NZ	LYS	D	722	125.623	3.789	25.462	1.00	31.59	D
	ATOM	9102	C	LYS	D	722	123.152	-1.376	26.621	1.00	25.54	D
	ATOM	9103	O	LYS	D	722	123.556	-2.161	25.765	1.00	24.73	D
35	ATOM	9104	N	GLY	D	723	121.936	-0.851	26.580	1.00	25.69	D
	ATOM	9105	CA	GLY	D	723	121.044	-1.201	25.497	1.00	25.26	D
	ATOM	9106	C	GLY	D	723	120.804	-2.694	25.431	1.00	27.03	D
	ATOM	9107	O	GLY	D	723	120.226	-3.287	26.342	1.00	28.21	D
	ATOM	9108	N	LYS	D	724	121.262	-3.313	24.350	1.00	28.66	D
40	ATOM	9109	CA	LYS	D	724	121.087	-4.752	24.144	1.00	29.79	D
	ATOM	9110	CB	LYS	D	724	120.590	-4.978	22.732	1.00	30.45	D
	ATOM	9111	CG	LYS	D	724	121.344	-4.146	21.713	1.00	32.48	D
	ATOM	9112	CD	LYS	D	724	122.379	-4.944	20.947	1.00	34.54	D
	ATOM	9113	CE	LYS	D	724	122.796	-4.163	19.693	1.00	36.42	D
45	ATOM	9114	NZ	LYS	D	724	123.789	-4.878	18.817	1.00	36.97	D
	ATOM	9115	C	LYS	D	724	122.373	-5.535	24.346	1.00	29.03	D
	ATOM	9116	O	LYS	D	724	122.417	-6.749	24.142	1.00	28.40	D
	ATOM	9117	N	THR	D	725	123.409	-4.820	24.759	1.00	28.23	D
	ATOM	9118	CA	THR	D	725	124.720	-5.400	24.964	1.00	27.95	D
50	ATOM	9119	CB	THR	D	725	125.784	-4.578	24.178	1.00	27.43	D
	ATOM	9120	OG1	THR	D	725	125.351	-4.417	22.821	1.00	26.72	D
	ATOM	9121	CG2	THR	D	725	127.134	-5.273	24.189	1.00	25.82	D
	ATOM	9122	C	THR	D	725	125.106	-5.460	26.443	1.00	27.90	D
	ATOM	9123	O	THR	D	725	124.891	-4.505	27.199	1.00	28.70	D

	ATOM	9124	N	LEU	D	726	125.682	-6.591	26.842	1.00	26.83	D
	ATOM	9125	CA	LEU	D	726	126.119	-6.806	28.213	1.00	24.94	D
	ATOM	9126	CB	LEU	D	726	125.126	-7.703	28.937	1.00	27.71	D
	ATOM	9127	CG	LEU	D	726	125.632	-8.393	30.211	1.00	29.98	D
5	ATOM	9128	CD1	LEU	D	726	126.114	-7.390	31.271	1.00	30.93	D
	ATOM	9129	CD2	LEU	D	726	124.478	-9.202	30.758	1.00	31.05	D
	ATOM	9130	C	LEU	D	726	127.485	-7.441	28.245	1.00	22.94	D
	ATOM	9131	O	LEU	D	726	127.673	-8.537	27.741	1.00	24.07	D
	ATOM	9132	N	VAL	D	727	128.436	-6.753	28.856	1.00	23.62	D
10	ATOM	9133	CA	VAL	D	727	129.798	-7.256	28.940	1.00	23.62	D
	ATOM	9134	CB	VAL	D	727	130.766	-6.218	28.377	1.00	24.57	D
	ATOM	9135	CG1	VAL	D	727	132.189	-6.737	28.490	1.00	28.26	D
	ATOM	9136	CG2	VAL	D	727	130.414	-5.939	26.896	1.00	22.22	D
	ATOM	9137	C	VAL	D	727	130.214	-7.625	30.360	1.00	21.59	D
15	ATOM	9138	O	VAL	D	727	129.738	-7.034	31.333	1.00	20.77	D
	ATOM	9139	N	ALA	D	728	131.106	-8.608	30.461	1.00	21.47	D
	ATOM	9140	CA	ALA	D	728	131.597	-9.084	31.751	1.00	21.74	D
	ATOM	9141	CB	ALA	D	728	130.593	-10.057	32.371	1.00	23.07	D
	ATOM	9142	C	ALA	D	728	132.952	-9.749	31.692	1.00	21.99	D
20	ATOM	9143	O	ALA	D	728	133.199	-10.624	30.846	1.00	17.98	D
	ATOM	9144	N	ALA	D	729	133.823	-9.315	32.605	1.00	24.10	D
	ATOM	9145	CA	ALA	D	729	135.175	-9.868	32.740	1.00	25.79	D
	ATOM	9146	CB	ALA	D	729	136.139	-8.792	33.225	1.00	26.49	D
	ATOM	9147	C	ALA	D	729	135.036	-10.980	33.770	1.00	26.20	D
25	ATOM	9148	O	ALA	D	729	134.619	-10.736	34.900	1.00	24.79	D
	ATOM	9149	N	VAL	D	730	135.363	-12.199	33.351	1.00	27.91	D
	ATOM	9150	CA	VAL	D	730	135.224	-13.396	34.182	1.00	28.52	D
	ATOM	9151	CB	VAL	D	730	134.162	-14.349	33.578	1.00	25.65	D
	ATOM	9152	CG1	VAL	D	730	132.846	-13.619	33.401	1.00	21.69	D
30	ATOM	9153	CG2	VAL	D	730	134.667	-14.910	32.251	1.00	23.86	D
	ATOM	9154	C	VAL	D	730	136.496	-14.215	34.373	1.00	30.60	D
	ATOM	9155	O	VAL	D	730	137.544	-13.945	33.773	1.00	29.25	D
	ATOM	9156	N	GLU	D	731	136.373	-15.227	35.224	1.00	34.05	D
	ATOM	9157	CA	GLU	D	731	137.468	-16.136	35.507	1.00	38.43	D
35	ATOM	9158	CB	GLU	D	731	138.069	-15.875	36.877	1.00	39.08	D
	ATOM	9159	CG	GLU	D	731	139.163	-16.851	37.195	1.00	41.06	D
	ATOM	9160	CD	GLU	D	731	139.469	-16.908	38.664	1.00	44.19	D
	ATOM	9161	OE1	GLU	D	731	139.986	-15.898	39.204	1.00	43.94	D
	ATOM	9162	OE2	GLU	D	731	139.184	-17.969	39.275	1.00	45.15	D
40	ATOM	9163	C	GLU	D	731	136.915	-17.541	35.481	1.00	39.52	D
	ATOM	9164	O	GLU	D	731	136.003	-17.862	36.239	1.00	38.90	D
	ATOM	9165	N	LYS	D	732	137.464	-18.375	34.606	1.00	42.02	D
	ATOM	9166	CA	LYS	D	732	137.000	-19.744	34.487	1.00	44.14	D
	ATOM	9167	CB	LYS	D	732	136.079	-19.864	33.279	1.00	45.79	D
45	ATOM	9168	CG	LYS	D	732	135.263	-21.130	33.269	1.00	48.52	D
	ATOM	9169	CD	LYS	D	732	134.329	-21.169	32.074	1.00	48.95	D
	ATOM	9170	CE	LYS	D	732	133.753	-22.555	31.897	1.00	50.73	D
	ATOM	9171	NZ	LYS	D	732	132.777	-22.576	30.795	1.00	53.14	D
	ATOM	9172	C	LYS	D	732	138.155	-20.724	34.366	1.00	45.13	D
50	ATOM	9173	O	LYS	D	732	139.012	-20.593	33.491	1.00	46.00	D
	ATOM	9174	N	ASP	D	733	138.179	-21.702	35.263	1.00	45.68	D
	ATOM	9175	CA	ASP	D	733	139.227	-22.710	35.263	1.00	45.99	D
	ATOM	9176	CB	ASP	D	733	139.114	-23.590	34.013	1.00	47.96	D
	ATOM	9177	CG	ASP	D	733	137.759	-24.322	33.917	1.00	51.97	D

	ATOM	9178	OD1	ASP	D	733	137.355	-24.977	34.905	1.00	55.70	D
	ATOM	9179	OD2	ASP	D	733	137.095	-24.256	32.855	1.00	50.55	D
	ATOM	9180	C	ASP	D	733	140.603	-22.066	35.311	1.00	45.97	D
	ATOM	9181	O	ASP	D	733	141.493	-22.456	34.565	1.00	46.45	D
5	ATOM	9182	N	GLY	D	734	140.778	-21.075	36.182	1.00	45.60	D
	ATOM	9183	CA	GLY	D	734	142.072	-20.420	36.295	1.00	44.79	D
	ATOM	9184	C	GLY	D	734	142.438	-19.447	35.182	1.00	44.98	D
	ATOM	9185	O	GLY	D	734	143.607	-19.089	35.012	1.00	44.45	D
	ATOM	9186	N	GLN	D	735	141.453	-19.010	34.411	1.00	43.41	D
10	ATOM	9187	CA	GLN	D	735	141.747	-18.067	33.349	1.00	42.41	D
	ATOM	9188	CB	GLN	D	735	141.935	-18.820	32.034	1.00	44.33	D
	ATOM	9189	CG	GLN	D	735	143.185	-19.679	32.036	1.00	46.62	D
	ATOM	9190	CD	GLN	D	735	143.303	-20.555	30.810	1.00	48.33	D
	ATOM	9191	OE1	GLN	D	735	143.228	-20.076	29.670	1.00	49.33	D
15	ATOM	9192	NE2	GLN	D	735	143.495	-21.853	31.035	1.00	48.62	D
	ATOM	9193	C	GLN	D	735	140.647	-17.025	33.243	1.00	40.32	D
	ATOM	9194	O	GLN	D	735	139.504	-17.282	33.609	1.00	40.35	D
	ATOM	9195	N	SER	D	736	141.001	-15.841	32.765	1.00	37.70	D
	ATOM	9196	CA	SER	D	736	140.033	-14.770	32.630	1.00	35.67	D
20	ATOM	9197	CB	SER	D	736	140.664	-13.454	33.051	1.00	35.55	D
	ATOM	9198	OG	SER	D	736	141.815	-13.209	32.262	1.00	33.28	D
	ATOM	9199	C	SER	D	736	139.580	-14.656	31.191	1.00	35.08	D
	ATOM	9200	O	SER	D	736	140.375	-14.823	30.273	1.00	35.01	D
	ATOM	9201	N	PHE	D	737	138.299	-14.370	30.998	1.00	35.00	D
25	ATOM	9202	CA	PHE	D	737	137.749	-14.215	29.662	1.00	34.26	D
	ATOM	9203	CB	PHE	D	737	136.928	-15.436	29.259	1.00	34.41	D
	ATOM	9204	CG	PHE	D	737	137.736	-16.689	29.121	1.00	34.85	D
	ATOM	9205	CD1	PHE	D	737	138.122	-17.416	30.243	1.00	34.24	D
	ATOM	9206	CD2	PHE	D	737	138.120	-17.140	27.864	1.00	34.84	D
30	ATOM	9207	CE1	PHE	D	737	138.871	-18.574	30.108	1.00	34.16	D
	ATOM	9208	CE2	PHE	D	737	138.868	-18.293	27.724	1.00	33.97	D
	ATOM	9209	CZ	PHE	D	737	139.246	-19.012	28.845	1.00	34.14	D
	ATOM	9210	C	PHE	D	737	136.869	-12.992	29.611	1.00	33.97	D
	ATOM	9211	O	PHE	D	737	136.627	-12.359	30.639	1.00	34.16	D
35	ATOM	9212	N	LEU	D	738	136.387	-12.673	28.411	1.00	32.98	D
	ATOM	9213	CA	LEU	D	738	135.526	-11.514	28.199	1.00	33.21	D
	ATOM	9214	CB	LEU	D	738	136.222	-10.527	27.255	1.00	32.13	D
	ATOM	9215	CG	LEU	D	738	135.744	-9.075	27.237	1.00	32.97	D
	ATOM	9216	CD1	LEU	D	738	134.465	-8.962	26.461	1.00	33.24	D
40	ATOM	9217	CD2	LEU	D	738	135.574	-8.569	28.668	1.00	33.16	D
	ATOM	9218	C	LEU	D	738	134.180	-11.955	27.620	1.00	33.76	D
	ATOM	9219	O	LEU	D	738	134.110	-12.360	26.473	1.00	36.66	D
	ATOM	9220	N	GLU	D	739	133.114	-11.870	28.410	1.00	33.64	D
	ATOM	9221	CA	GLU	D	739	131.793	-12.292	27.959	1.00	32.51	D
45	ATOM	9222	CB	GLU	D	739	131.000	-12.884	29.121	1.00	33.25	D
	ATOM	9223	CG	GLU	D	739	131.529	-14.166	29.668	1.00	34.95	D
	ATOM	9224	CD	GLU	D	739	131.644	-15.235	28.602	1.00	38.68	D
	ATOM	9225	OE1	GLU	D	739	130.731	-15.323	27.733	1.00	38.32	D
	ATOM	9226	OE2	GLU	D	739	132.651	-15.991	28.646	1.00	39.63	D
50	ATOM	9227	C	GLU	D	739	130.961	-11.163	27.377	1.00	32.88	D
	ATOM	9228	O	GLU	D	739	130.735	-10.144	28.044	1.00	33.94	D
	ATOM	9229	N	ILE	D	740	130.487	-11.329	26.147	1.00	31.70	D
	ATOM	9230	CA	ILE	D	740	129.641	-10.301	25.568	1.00	29.64	D
	ATOM	9231	CB	ILE	D	740	130.288	-9.670	24.299	1.00	28.27	D

	ATOM	9232	CG2	ILE	D	740	129.461	-8.484	23.831	1.00	27.08	D
	ATOM	9233	CG1	ILE	D	740	131.663	-9.093	24.620	1.00	24.97	D
	ATOM	9234	CD1	ILE	D	740	132.282	-8.385	23.424	1.00	24.47	D
	ATOM	9235	C	ILE	D	740	128.275	-10.906	25.252	1.00	29.65	D
5	ATOM	9236	O	ILE	D	740	128.174	-11.845	24.470	1.00	30.71	D
	ATOM	9237	N	LEU	D	741	127.226	-10.388	25.885	1.00	30.03	D
	ATOM	9238	CA	LEU	D	741	125.872	-10.903	25.659	1.00	30.25	D
	ATOM	9239	CB	LEU	D	741	125.209	-11.213	26.994	1.00	30.19	D
	ATOM	9240	CG	LEU	D	741	126.016	-12.176	27.872	1.00	30.17	D
10	ATOM	9241	CD1	LEU	D	741	125.458	-12.120	29.284	1.00	31.69	D
	ATOM	9242	CD2	LEU	D	741	125.969	-13.591	27.323	1.00	26.90	D
	ATOM	9243	C	LEU	D	741	125.012	-9.935	24.863	1.00	29.80	D
	ATOM	9244	O	LEU	D	741	124.939	-8.750	25.176	1.00	28.77	D
	ATOM	9245	N	ASP	D	742	124.354	-10.462	23.837	1.00	31.56	D
15	ATOM	9246	CA	ASP	D	742	123.513	-9.664	22.948	1.00	32.74	D
	ATOM	9247	CB	ASP	D	742	123.917	-9.906	21.492	1.00	33.83	D
	ATOM	9248	CG	ASP	D	742	123.601	-8.730	20.592	1.00	34.30	D
	ATOM	9249	OD1	ASP	D	742	122.422	-8.315	20.526	1.00	33.76	D
	ATOM	9250	OD2	ASP	D	742	124.550	-8.223	19.952	1.00	34.48	D
20	ATOM	9251	C	ASP	D	742	122.046	-10.021	23.110	1.00	33.39	D
	ATOM	9252	O	ASP	D	742	121.617	-11.102	22.713	1.00	33.45	D
	ATOM	9253	N	PHE	D	743	121.283	-9.097	23.685	1.00	34.50	D
	ATOM	9254	CA	PHE	D	743	119.858	-9.296	23.905	1.00	34.56	D
	ATOM	9255	CB	PHE	D	743	119.422	-8.544	25.161	1.00	32.05	D
25	ATOM	9256	CG	PHE	D	743	119.627	-9.324	26.400	1.00	29.59	D
	ATOM	9257	CD1	PHE	D	743	120.893	-9.462	26.941	1.00	27.43	D
	ATOM	9258	CD2	PHE	D	743	118.579	-10.058	26.935	1.00	28.98	D
	ATOM	9259	CE1	PHE	D	743	121.116	-10.332	27.987	1.00	26.97	D
	ATOM	9260	CE2	PHE	D	743	118.787	-10.933	27.980	1.00	27.93	D
30	ATOM	9261	CZ	PHE	D	743	120.059	-11.077	28.507	1.00	26.94	D
	ATOM	9262	C	PHE	D	743	118.973	-8.895	22.734	1.00	35.12	D
	ATOM	9263	O	PHE	D	743	117.746	-8.889	22.849	1.00	35.80	D
	ATOM	9264	N	SER	D	744	119.594	-8.592	21.600	1.00	35.35	D
	ATOM	9265	CA	SER	D	744	118.854	-8.176	20.416	1.00	35.76	D
35	ATOM	9266	CB	SER	D	744	119.823	-7.612	19.381	1.00	36.40	D
	ATOM	9267	OG	SER	D	744	119.126	-6.857	18.417	1.00	40.54	D
	ATOM	9268	C	SER	D	744	118.029	-9.301	19.793	1.00	35.75	D
	ATOM	9269	O	SER	D	744	118.433	-10.488	19.873	1.00	36.28	D
	ATOM	9270	OXT	SER	D	744	116.984	-8.972	19.209	1.00	34.82	D
40	ATOM	9271	CB	LEU	E	2	57.203	-3.013	76.696	1.00	93.40	E
	ATOM	9272	CG	LEU	E	2	56.802	-2.909	78.154	1.00	92.64	E
	ATOM	9273	CD1	LEU	E	2	56.089	-4.209	78.494	1.00	92.62	E
	ATOM	9274	CD2	LEU	E	2	58.002	-2.716	79.063	1.00	91.70	E
	ATOM	9275	C	LEU	E	2	58.910	-2.837	74.950	1.00	94.06	E
45	ATOM	9276	O	LEU	E	2	59.052	-4.056	75.064	1.00	94.80	E
	ATOM	9277	N	LEU	E	2	57.498	-0.813	75.549	1.00	93.79	E
	ATOM	9278	CA	LEU	E	2	58.180	-2.054	76.029	1.00	93.74	E
	ATOM	9279	N	LEU	E	3	59.349	-2.162	73.890	1.00	93.32	E
	ATOM	9280	CA	LEU	E	3	60.093	-2.853	72.840	1.00	91.84	E
50	ATOM	9281	CB	LEU	E	3	60.099	-2.030	71.539	1.00	90.21	E
	ATOM	9282	CG	LEU	E	3	58.738	-2.011	70.818	1.00	88.51	E
	ATOM	9283	CD1	LEU	E	3	58.863	-1.419	69.431	1.00	86.61	E
	ATOM	9284	CD2	LEU	E	3	58.194	-3.426	70.729	1.00	87.78	E
	ATOM	9285	C	LEU	E	3	61.504	-3.132	73.355	1.00	91.93	E

	ATOM	9286	O	LEU	E	3	62.459	-2.428	73.011	1.00	92.22	E
	ATOM	9287	N	TPO	E	4	61.634	-4.171	74.204	1.00	91.56	E
	ATOM	9288	CA	TPO	E	4	62.536	-4.975	75.032	1.00	90.52	E
	ATOM	9289	CB	TPO	E	4	62.853	-4.058	76.249	1.00	89.37	E
5	ATOM	9290	CG2	TPO	E	4	63.717	-4.740	77.314	1.00	89.39	E
	ATOM	9291	OG1	TPO	E	4	63.546	-2.864	75.833	1.00	86.87	E
	ATOM	9292	P	TPO	E	4	65.016	-2.884	75.092	1.00	83.35	E
	ATOM	9293	O1P	TPO	E	4	64.849	-3.624	73.731	1.00	83.36	E
	ATOM	9294	O2P	TPO	E	4	66.088	-3.641	76.006	1.00	83.80	E
10	ATOM	9295	O3P	TPO	E	4	65.359	-1.340	74.831	1.00	84.80	E
	ATOM	9296	C	TPO	E	4	61.804	-6.259	75.507	1.00	91.34	E
	ATOM	9297	O	TPO	E	4	60.467	-6.316	75.619	1.00	91.46	E
	ATOM	9298	N	PRO	E	5	63.256	-5.997	71.948	1.00	83.51	E
	ATOM	9299	CD	PRO	E	5	63.441	-4.606	71.529	1.00	83.14	E
15	ATOM	9300	CA	PRO	E	5	63.931	-6.885	71.003	1.00	84.53	E
	ATOM	9301	CB	PRO	E	5	65.159	-6.089	70.575	1.00	83.61	E
	ATOM	9302	CG	PRO	E	5	64.831	-4.637	70.919	1.00	83.06	E
	ATOM	9303	C	PRO	E	5	64.316	-8.236	71.564	1.00	85.50	E
	ATOM	9304	O	PRO	E	5	64.916	-8.330	72.628	1.00	85.67	E
20	ATOM	9305	N	PRO	E	6	63.969	-9.312	70.847	1.00	86.93	E
	ATOM	9306	CD	PRO	E	6	63.085	-9.303	69.669	1.00	87.22	E
	ATOM	9307	CA	PRO	E	6	64.267	-10.690	71.255	1.00	88.33	E
	ATOM	9308	CB	PRO	E	6	63.629	-11.522	70.149	1.00	87.80	E
	ATOM	9309	CG	PRO	E	6	62.478	-10.688	69.722	1.00	87.62	E
25	ATOM	9310	C	PRO	E	6	65.765	-10.988	71.384	1.00	89.85	E
	ATOM	9311	O	PRO	E	6	66.575	-10.544	70.557	1.00	90.61	E
	ATOM	9312	N	GLN	E	7	66.126	-11.745	72.421	1.00	90.83	E
	ATOM	9313	CA	GLN	E	7	67.515	-12.125	72.626	1.00	91.45	E
	ATOM	9314	CB	GLN	E	7	68.006	-11.682	73.992	1.00	91.16	E
30	ATOM	9315	CG	GLN	E	7	68.555	-10.282	73.957	1.00	91.12	E
	ATOM	9316	CD	GLN	E	7	69.842	-10.165	74.739	1.00	91.14	E
	ATOM	9317	OE1	GLN	E	7	69.851	-10.287	75.975	1.00	92.25	E
	ATOM	9318	NE2	GLN	E	7	70.950	-9.958	74.025	1.00	89.30	E
	ATOM	9319	C	GLN	E	7	67.666	-13.631	72.485	1.00	91.90	E
35	ATOM	9320	O	GLN	E	7	67.429	-14.383	73.431	1.00	92.11	E
	ATOM	9321	N	SER	E	8	68.051	-14.055	71.282	1.00	92.25	E
	ATOM	9322	CA	SER	E	8	68.235	-15.467	70.933	1.00	92.14	E
	ATOM	9323	CB	SER	E	8	67.113	-15.896	69.981	1.00	92.25	E
	ATOM	9324	OG	SER	E	8	66.978	-17.305	69.938	1.00	92.67	E
40	ATOM	9325	C	SER	E	8	69.603	-15.640	70.258	1.00	92.02	E
	ATOM	9326	O	SER	E	8	70.638	-15.398	70.879	1.00	91.94	E
	ATOM	9327	N	GLY	E	9	69.602	-16.057	68.994	1.00	91.78	E
	ATOM	9328	CA	GLY	E	9	70.854	-16.235	68.277	1.00	91.39	E
	ATOM	9329	C	GLY	E	9	70.848	-15.537	66.928	1.00	91.23	E
45	ATOM	9330	O	GLY	E	9	69.743	-15.212	66.445	1.00	90.99	E
	ATOM	9331	OXT	GLY	E	9	71.939	-15.322	66.346	1.00	90.21	E
	ATOM	9332	CB	LEU	F	2	137.489	-5.702	48.818	1.00	79.71	F
	ATOM	9333	CG	LEU	F	2	138.842	-5.743	49.546	1.00	80.18	F
	ATOM	9334	CD1	LEU	F	2	139.667	-4.549	49.099	1.00	79.66	F
50	ATOM	9335	CD2	LEU	F	2	138.661	-5.730	51.075	1.00	78.72	F
	ATOM	9336	C	LEU	F	2	138.487	-6.493	46.630	1.00	78.95	F
	ATOM	9337	O	LEU	F	2	138.336	-7.720	46.632	1.00	77.64	F
	ATOM	9338	N	LEU	F	2	136.056	-5.715	46.790	1.00	79.28	F
	ATOM	9339	CA	LEU	F	2	137.454	-5.545	47.286	1.00	79.36	F

5	ATOM	9340	N	LEU	F	3	139.520	-5.871	46.060	1.00	78.25	F
	ATOM	9341	CA	LEU	F	3	140.670	-6.502	45.403	1.00	76.54	F
	ATOM	9342	CB	LEU	F	3	140.433	-6.740	43.915	1.00	77.32	F
	ATOM	9343	CG	LEU	F	3	139.459	-7.802	43.429	1.00	78.88	F
	ATOM	9344	CD1	LEU	F	3	138.100	-7.190	43.081	1.00	80.14	F
10	ATOM	9345	CD2	LEU	F	3	140.065	-8.449	42.204	1.00	78.71	F
	ATOM	9346	C	LEU	F	3	141.723	-5.415	45.530	1.00	75.20	F
	ATOM	9347	O	LEU	F	3	141.444	-4.264	45.195	1.00	75.82	F
	ATOM	9348	N	TPO	F	4	142.936	-5.746	46.012	1.00	72.87	F
	ATOM	9349	CA	TPO	F	4	144.008	-4.734	46.163	1.00	70.82	F
15	ATOM	9350	CB	TPO	F	4	144.161	-4.534	47.709	1.00	68.53	F
	ATOM	9351	CG2	TPO	F	4	145.393	-3.748	48.146	1.00	70.46	F
	ATOM	9352	OG1	TPO	F	4	142.965	-3.903	48.203	1.00	65.51	F
	ATOM	9353	P	TPO	F	4	142.778	-2.260	48.081	1.00	60.19	F
	ATOM	9354	O1P	TPO	F	4	142.871	-1.889	46.565	1.00	64.16	F
20	ATOM	9355	O2P	TPO	F	4	143.905	-1.501	48.889	1.00	62.63	F
	ATOM	9356	O3P	TPO	F	4	141.319	-1.975	48.672	1.00	64.49	F
	ATOM	9357	C	TPO	F	4	145.311	-5.244	45.579	1.00	70.94	F
	ATOM	9358	O	TPO	F	4	145.629	-6.541	45.562	1.00	71.31	F
	ATOM	9359	N	PRO	F	5	146.116	-4.278	45.081	1.00	71.04	F
25	ATOM	9360	CD	PRO	F	5	145.651	-2.886	44.895	1.00	69.22	F
	ATOM	9361	CA	PRO	F	5	147.434	-4.439	44.468	1.00	71.37	F
	ATOM	9362	CB	PRO	F	5	147.722	-3.051	43.898	1.00	70.57	F
	ATOM	9363	CG	PRO	F	5	146.379	-2.473	43.673	1.00	68.58	F
	ATOM	9364	C	PRO	F	5	148.447	-4.823	45.533	1.00	72.63	F
30	ATOM	9365	O	PRO	F	5	148.273	-4.524	46.709	1.00	72.26	F
	ATOM	9366	N	PRO	F	6	149.531	-5.484	45.133	1.00	74.58	F
	ATOM	9367	CD	PRO	F	6	149.883	-5.888	43.760	1.00	74.65	F
	ATOM	9368	CA	PRO	F	6	150.563	-5.898	46.087	1.00	76.44	F
	ATOM	9369	CB	PRO	F	6	151.636	-6.499	45.180	1.00	76.17	F
35	ATOM	9370	CG	PRO	F	6	150.843	-7.015	44.005	1.00	75.36	F
	ATOM	9371	C	PRO	F	6	151.108	-4.721	46.907	1.00	78.12	F
	ATOM	9372	O	PRO	F	6	151.745	-3.827	46.351	1.00	78.87	F
	ATOM	9373	N	GLN	F	7	150.858	-4.699	48.213	1.00	79.62	F
	ATOM	9374	CA	GLN	F	7	151.397	-3.605	49.020	1.00	81.37	F
40	ATOM	9375	CB	GLN	F	7	150.607	-3.435	50.333	1.00	81.68	F
	ATOM	9376	CG	GLN	F	7	151.014	-2.213	51.171	1.00	82.68	F
	ATOM	9377	CD	GLN	F	7	150.936	-0.896	50.397	1.00	83.36	F
	ATOM	9378	OE1	GLN	F	7	151.562	-0.740	49.343	1.00	84.22	F
	ATOM	9379	NE2	GLN	F	7	150.175	0.061	50.927	1.00	82.82	F
45	ATOM	9380	C	GLN	F							

Table 7.
Oligonucleotides used in Example 2

MTO#	Oligo name	Sequence
MTO 1146	LP6DelA-FWD	gccttcgcgaactgatgtacactttgcagggtcatacagc
MTO 1147	LP6DelA-REV	gccttggccattttctagatcccaattctaatagtggtatccatac
MTO 1254	CDC4-BNSH-F	gtaggatccatatggcgccgcaagcttcccttagctgagttcc
MTO 1367	V384N-C	catatgacgagtaataattacgtgcttgc
MTO 1368	V384N3	caagcacgtaataattactcgcatatg
MTO 1369	K402A-C	ggggctgatgacgcaatgatcagag
MTO 1370	K402A-N	ctctgatcattgcgtcatcagcccc
MTO 1371	W426A 5'	gatgggtgggttgcggcgtgaagtatgcccatg
MTO 1372	DN426A	catgggcatacttcagcgccgcaacccaccatc
MTO 1373	R443D-C	ggttctacagacgacacgggtccgagtttggg
MTO 1374	R443D	tatcccaaactcggaccgtgtcgtcgtctgtagaaccg
MTO 1375	Y548F	cagtgtattatcaaaagcttcactaacgac
MTO 1376	Y548F-C	gtcgttagtgaagctttgataataactg
MTO 1377	Y574F-N	gtagattgtcgaataatttcgatcgtatg
MTO 1378	Y574F-C	catacggatcgaatattttcgacaatctac
MTO 1379	W717N Hpa	ttgcccttaaagttaaccgagttaatctgatcag
MTO 1380	W717N-C	ctgatcagattaactcggtaactttaagggcaa
MTO 1381	2Flex359 5'	tcttttctggagcccgcccaattttaaaaaattggtac
MTO 1382	2Flex359 3'	gtaccaatttttaaaattggcccggtccagaaaaga
MTO 1383	H5 Dest 5'	ggttttaattctctcgcccgccgacctccaaaaataccaaaaactc
MTO 1384	H5 Dest 3'	gagtttgggtatttttgggaggggtcccgccgagagaattaaaacc
MTO 1385	H5 del 5'	gtgagcccaaaagggtccaaagctttcacaacaagatcgc
MTO 1386	H5 del 3'	gcgatcttgttgtaaagctttggaccctttgggtcac
MTO 1387	H5+ Dest 5'	gtggaaaaaactctgatattcattttaaaaaattggtacaatcc
MTO 1388	H5+ Dest 3'	ggattgtaccaatttttaaaatgaatatcagaagttttccac
MTO 1389	Ala1-3	ccaatttttaaaatgaatgcaatattctccagaaaag
MTO 1390	Ala2-3	ccaatttttaaaatgaatgctgcaatattctccagaaaag
MTO 1391	Ala3-3	ccaatttttaaaatgaagcggctgcaatattctccagaaaag
MTO 1392	Ala4-3	ccaatttttaaaatgaaggctgcagctgcaatattctccagaaaag
MTO 1393	Ala8 5'	gccgcgcgcgctaaagctgcagcgttcattttaaaaaattggtacaatcc
MTO 1394	Ala8 3'	cgctgcagcttagcgcgcgcggctatattctccagaaaagataatc
MTO 1395	Ala12 5'	gccgcgcgcgctaaagctgcagcgcgcgcgaaagccttcattttaaaaaattggtacaatcc
MTO 1396	Ala12 3'	ggctttcgcgcgcgctgcagcttagcgcgcgcggctatattctccagaaaagataatc

Table 8.
Plasmids used in Example 2

Plasmid	Relevant Characteristic	Source
pMT 3169	pProEx Hta-CDC4 LP6DeIA GST-Skp1	This study
pMT 3055	pProEx Hta-CDC4 263-744 GST-Skp1	Nash et. al.
pMT 3000	pProEx Hta-CDC4 1-744 GST-Skp1	This study
pMT 3217	pRS 314 CDC4-BNSH/Eco	This study
pMT 3001	pMT 3055 V384N	This study
pMT 3002	pMT 3055 K402A	This study
pMT 3385	pMT 3055 W426A	This study
pMT 3058	pMT 3055 R443A	Nash et. al
pMT 3003	pMT 3055 R443D	This study
pMT 3059	pMT 3055 R467A	Nash et. al
pMT 3060	pMT 3055 R485A	Nash et. al
pMT 3061	pMT 3055 R534A	Nash et. al
pMT 3004	pMT 3055 Y548F	This study
pMT 3005	pMT 3055 Y574F	This study
pMT 3006	pMT 3055 W717N	This study
pMT 3007	pMT 3055 V384N+W717N	This study
pMT 3008	pMT 3055 K402+R443D	This study
pMT 3010	pMT 3000 R443D	This study
pMT 3011	pMT 3000 R443A	This study
pMT 3012	pMT 3000 W717N	This study
pMT 3013	pMT 3000 K402A+R443D	This study
pMT 3014	pMT 3000 V384N+W717N	This study
pMT 3015	pMT 3217 V384N	This study
pMT 3016	pMT 3217 K402A	This study
pMT 3386	pMT 3217 W426A	This study
pMT 3017	pMT 3217 R443D	This study
pMT 3058	PRS 314-CDC4 R443A	Nash et. al.
pMT 3018	pMT 3217 Y548F	This study
pMT 3068	PRS 314-CDC4 R572A	Nash et. al
pMT 3019	pMT 3217 Y574F	This study
pMT 3020	pMT 3217 W717N	This study
pMT 3021	pMT 3217 V384N+W717N	This study
pMT 3022	pMT 3217 K402A+R443D	This study
pMT 3024	pMT 3000 Helix 5 Δ 330-443	This study
pMT 3025	pMT 3000 Helix 5 breaker	This study
pMT 3026	pMT 3000 Helix 5 Δ 321-360	This study
pMT 3027	pMT 3000 Helix 6 breaker	This study
pMT 3028	pMT 3000 Ala1 insert	This study
pMT 3029	pMT 3000 Ala2 insert	This study
pMT 3030	pMT 3000 Ala3 insert	This study
pMT 3031	pMT 3000 Ala4 insert	This study
pMT 3032	pMT 3000 Ala8 insert	This study
pMT 3033	pMT 3000 Ala12 insert	This study
pMT 3034	pMT 3217 Helix 5 Δ 330-443	This study
pMT 3035	pMT 3217 Helix 5 breaker	This study
pMT 3036	pMT 3217 Helix 5 Δ 321-360	This study

Plasmid	Relevant Characteristic	Source
pMT 3037	pMT 3217 Helix 6 breaker	This study
pMT 3038	pMT 3217 Ala1 insert	This study
pMT 3039	pMT 3217 Ala2 insert	This study
pMT 3040	pMT 3217 Ala3 insert	This study
pMT 3041	pMT 3217 Ala4 insert	This study
pMT 3042	pMT 3217 Ala8 insert	This study
pMT 3043	pMT 3217 Ala12 insert	This study
pMT 1571	Pet16b-Sic1	Previous study
MDM 152	pGAL11 SIC1 LEU2 CEN ARS	M. Mendenhall
MDM202	pGAL1 SIC1 ^{T33V} LEU2 CEN ARS	M. Mendenhall

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